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Dr. Henry A. Resing

(May 23, 1933 – December 22, 1988)

Although Dr. Resing took up his place as ONREUR's Liaison Scientist for Chemistry only six months ago, he was already in the full swing of his job, had set all the wheels in motion, and was reaping the fruit of his thorough and vigorous preparations when he was stricken by a fatal heart attack. It happened while he was on the job – at the University of Nottingham, where he was attending a conference.

He had very quickly established himself in our office not only as a hard-driving professional but also as an extraordinarily likeable man, at once serious and easily amused – enjoying the puzzles of the physical world as well as the humor implicit in human affairs. That may be why he was so especially likeable.

Long before he checked into our office he laid the groundwork for a running start: within a week of his arrival – even while his new household was being established – he was off to Norway and within a month of his arrival here was attending a five-day conference in West Germany, reaping the payoff for the extra work he had put in before and during the closeout of his affairs at the Naval Research Laboratory.

He began making phone calls to his other UK and continental colleagues the first day he was in the office – letting them know he was now located in Europe, and setting up appointments, getting references to other people and institutions doing noteworthy work, and establishing (or extending) the boundaries of his technical and geographic turf. He knew what he was going to do as soon as he arrived, and he began to do it immediately.

Since arranging for visits normally involves long lead times, especially to destinations on the continent, many of Dr. Resing's first visits were to people and institutions in the UK. His articles, beginning on page 1, reflect, in part, this fact of the Liaison Scientist's life, but in the notes he left was the material for several more articles that he would have written on his return to the office. That he died on the steps of the conference meeting hall, in the very midst of gathering information, speaks clearly of his dedication.

Despite the seldom relaxed concentration on his work (he was very often the last person to leave the office) Dr. Resing soon became a most welcome and much appreciated personality in the office setting. His wry comments, his quickness to see a humorous irony, his appreciation of the banter at lunch, and the frequent and pleasant chuckle that signalled his thoroughly appreciative response to people endeared him to everyone.

Losing him was, of course, a severe shock, and a deep sense of personal loss is shared by all of us at ONREUR. Losing him is also a severe loss to the readers of ESNIB: Dr. Resing had only begun.

for the ONREUR staff,
C.J. Fox

ESN INFORMATION BULLETIN

89-01

This publication is approved for official dissemination of technical and scientific information of interest to the Defense research community and the scientific community at large

Commanding Officer ..... CAPT Terry J. McCloskey, USN
Scientific Director ..... James E. Andrews
Editor ..... C.J. Fox

Office of Naval Research European Office

With this issue, the first in 1989, we begin to use our new Command designation: the Office of Naval Research European Office. The designator was changed by command in December 1988 to more accurately reflect the geographic scope of our reporting and liaison functions. Our new abbreviated designator is ONREUR.

CHEMISTRY

Selected presentations given at the 12th International Liquid Crystal Conference, held in August 1988 at Freiburg, West Germany, are highlighted. This review is organized under the topics of: applications, synthesis, dynamics and order, and phase structure.

The work of various investigators at the UK's University of Kent is discussed. There is considerable concentration by the Kent investigators on the properties of solids and liquids in their finely divided state. Work includes structural studies of solids and liquids in their finely divided states, NMR studies into absorbed alcohol and short chains hydrocarbons, and computation simulation of the structure and dynamics of finely divided liquids.

Although the emphasis in this meeting, held in April 1988 at Bristol, UK, was on zeolite catalysts and lyotropic liquid crystals, a full range of interfacial phenomena were covered. Selected presentations are reviewed.

Work at the University of London Imperial College of Science and Technology in chemistry of zeolites is reviewed. This work includes study of the method of separation of petrochemical mixtures, examining the different methods of measuring diffusion coefficients within the pores or channels of zeolite crystals, and research into the binding of properties of radioactive actinide ions in clay.

AERONAUTICS

COMPUTER SCIENCE

MATERIALS SCIENCE/SEMICONDUCTORS

MATHEMATICS

PHYSICS

CHEMISTRY

The Twelfth International Liquid Crystal Conference

by Henry A. Resing.

The centenary of the discovery of liquid crystals by Otto Lehmann, a native son of Freiburg (West Germany), was celebrated appropriately in Freiburg through the 12th International Liquid Crystal Conference, 15 through 19 August 1988. The 500 papers and 700 attendees made the conference at once multidisciplinary, basic, applied, sharply focused, wide ranging, well organized, and explosive. The disciplines were organic chemistry, polymer science, physical chemistry, electrical engineering, solid-state (low-dimensional) physics and optoelectronics.

Applications

The liquid crystal application of transcendent interest is for panel displays, namely the replacement of cathode ray tubes by less bulky, lower energy, lighter weight "LC" displays. What long stood in the way was the requirement of one wire per pixel; the problem has been ameliorated by so-called multiplexing, which requires only one wire for every row and another for every column. Video rates have been achieved. Miniature (5-inch diagonal) color TV sets are in production – scheduled for "individual" airline passenger entertainment by a US airline. As one speaker pointed out: "Another example of a technology discovered in Europe, developed in the US, and commercialized in Japan."

Display devices have been made using some eight different electro-optical effects. To a high degree these are electrochemical effects. The chemical issues are: degrees and rates of alignment of molecules by electric fields; temperature regimes of existence for phases which allow such effects; discovery of new and better LC phases; a necessary alignment of molecules by the glass plates which bound the LC film in a device; and development of liquid crystalline polymers which may be similarly useful in devices and be free standing, thus not requiring bounding glass plates. And then there is the overriding need for basic understanding of LC's in general. My bias lies in the latter area, in using nuclear magnetic resonance (NMR) spectroscopy to measure molecular ordering, and thereby to strengthen the physicochemical basis for construction of such devices.

Synthesis

In the opening lecture Professor P. Demus (University of Halle, West Germany) viewed liquid crystal molecules as assemblies of rigid rods, flexible spacers, long chains, polar groups, discotic groups, and pyramidal groups. These groups may be linked together in various combinations and in various positions to provide new liquid crystaline materials. Even if such molecules themselves are not LC's, solutions of them with smaller space-filling molecules may generate new LC phases.

Such an explosion in the possible number of LC molecules due merely to "combinatorial" possibilities was extended in principle to infinity by Professor H. Ringsdorf (University of Mainz, West Germany) in his summary lecture; he linked Professor Demus' "units" in various repetition schemes to generate LC polymers. The polymers are indeed LC in many cases because the mesogenic units, linked by flexible hydrocarbon chains, nevertheless stack in columns or layers of less than three-dimensional order. The mesogenic units may be aromatic charge transfer partners; novel conducting polymers may result. Dye molecules may intercalate the ordered stacks and be held in dilute ordered arrays; new optical effects may result. Ringsdorf was able to bring Kevlar-like molecules into solution by suitable modification of the monomers with hydrophilic side chains. The resulting boardlike molecules earned themselves the Greek-rooted name "sanidic," which was said to be a new type of order in LC polymers. A stimulating lecture.

Dynamics and Order

For a uniaxial phase a useful order parameter, S, is the average value of the function

$$P_2 = \frac{(3\cos^2\theta - 1)}{2}$$

where θ is the angle between the unique axis and some accessible axis (i.e., an interproton vector) in the molecule. Although such an order parameter has long been available from splittings in NMR spectra, S is only a single term in the expansion of the distribution in θ in spherical

harmonics; many distributions in θ are compatible with a given S. This condition is unfortunately inherent in the rapidity of molecular rotation and diffusion in LC's. H. W. Spiess (MPI for Polymer Research, Mainz) has long sought to find the "full distribution" in θ and has succeeded in two cases. In LC polymeric glasses molecular motion is slower than in LC's and the two-dimensional (2-D) NMR spectrum for a certain selectively deuterated functional group yields the distribution in θ according to an analytical procedure which Spiess and H. Sillescu (also from MPI) worked out several years ago. Second, for LC's themselves, Spiess' group invented the experiment of following the spectrum in time after producing a non-equilibrium, inhomogeneous distribution of order parameters (by subjecting the sample to a pulse of magnetic torque). The spectra as functions of time, according to an analysis they developed, characterize the relaxation to equilibrium in terms of Leslie viscosity coefficients.

A nice example of the power of 2-D NMR as applied to LC polymers was given in the paper of K. Kohlhammer et al. (University of Stuttgart, West Germany) together with the Ringsdorf group concerning a polymer with rodlike elements in the main chain (with hexyloxy spacers) from which long hexyl chains terminated in rodlike elements. These were selectively deuterated in representative positions; spectra and thermal relaxation times, T, were measured:

- Deuterated para-linked phenyl rings on the main chain (spectra require ring flips to be rapid, and the thermal relaxation time, T_1, measures the rate of the flipping process)
- deuterated phenyl rings on the main chain to which side chains are attached (spectra show no flipping, T_1 measures rate of rocking vibration)
- deuterated para-linked phenyl groups in side chain (spectra show fast flipping, T_1 gives rate).

In addition, the transverse relaxation time is a measure of backbone reptation rates, which showed the expected precipitous fall (or equivalently, a steep rise in activation energy) as the glass temperature was approached. The glass transition did not affect the activation energy for the ring-flipping processes however. The spectra were analyzed as well for the orientation distribution as discussed above. The point here is that a rather simple experiment gives a great deal of information concerning molecular dynamics. The most difficult part is the provision of deuterated polymers, and it is only by collaboration with a synthetic group – i.e., that of Ringsdorf – that such progress is possible.

Paul Ukleja (Southwest Massachusetts State University, New Bedford) presented NMR linewidth and relaxation measurements for one of the few cubic liquid crystalline phases (work done on sabbatical at the Naval Research Laboratory). The structure of such phases is one of the true mysteries of liquid crystal science; how can there be a stiff, long-range ordered cubic structure in a temperature range between those of two smectic phases? The NMR spectroscopy revealed very fast molecular rotation (effectively isotropic) and diffusion. Such mysteries earned Ukleja some 70 reprint requests.

The embarrassment of riches provided by NMR leads to the paradox that there is no such thing as *the* molecular order parameter; rather there are many, each corresponding to a separate, in itself rigid, part or group of a flexible molecule. Now if these group-order parameters would scale with one another as temperature, pressure, or solvent (in a two-compound LC) and were varied, the concept of a single-order parameter might be rescued. In a study of solvent effects, G. L. Hoaston et al. (College of William & Mary, Williamsburg, Virginia) showed that such scaling does not occur. As far as NMR studies are concerned, there is no such thing as a molecular order parameter!

Phase Structure

R. Shashidar (Raman Research Institute, Bangalore, India) reviewed the various possible smectic A phases in terms of molecular "length." The layer of A2 is two molecules thick; A is one; Ad is incommensurate between one and two; $\bar{A}$ (antiphase) has a head group orientation which alternates, in any given layer, with a square wave periodicity; in Ac (A crenelated) the antiphase regions are of unequal length. Here we have an explosion in the possible number of phases due to the number of components and due to the variety of possible structures. Many of these phases only occur in binary systems, and the phase transitions on a temperature composition diagram must be theoretically understood, a process which is only now beginning. An example of such theory was given by A. Aharony (Tel Aviv University, Israel), who defined a suitable order parameter for the Hexatic B phase, showed how that order parameter might be measured by low-angle (synchrotron) X-ray scattering, and showed it to be calculable on the basis of standard solid-state theory for phase changes and critical phenomena, such as was generated for low-dimensional magnetic materials. The talk was so lucid, I believed for a while that I fully understood the matter.

Liquid crystals were discovered by means of optical microscopy. Georges Friedel showed that the textures observed through a polarizing microscope could only be generated through threadlike arrangements (nematic) or layerlike arrangements (smectic) of molecules. Yet such relations of texture to structure are not at all obvious. It was gratifying to find therefore that M. E. Neubert (Kent State University, Ohio) has generated a video text-book in which such textures and the phase changes related to change in texture are presented in a highly understandable way.

Summary

Clearly, only a few of the 500 papers have been touched upon. I found the applications papers to be so sharply focused that only an insider had any chance of taking the message away. An exception was the concluding lecture of the meeting by T. Carlson (Chalmers University of Technology, Sweden) delineating the requirements (successfully met) for displays based on ferroelectric liquid crystals; this talk is echoed somewhat in the introduction above. So the meeting, well-arranged by Professor Meier and his committee, celebrated an anniversary, explored the history of LC's, and gave the current status of this rapidly developing field.

The final "explosion" is that shown by the journal *Liquid Crystals*, which has gone from six issues per year in 1986 to a planned 18 in 1989. Of course six of these will carry the conference proceedings.

Finally, I am glad to say there is hope for me relative to understanding more about the complexities of LC's. Professor T. Riste (Institute for Energiteknikk, Kjeller, Norway) and Professor D. Sherrington (Imperial College, London) are organizing a NATO Advanced Study Institute (ASI) on "Phase Transitions in Soft Condensed Matter" (which includes liquid crystals) from 4 through 14 April 1989 in Geilo, Norway.

Similarly, G.R. Luckhurst (University of Southampton) and C.A. Veracini (University of Pisa) have been involved in organizing the NATO-ASI on the "Molecular Dynamics of Liquid Crystals" in Il Ciocco, Italy, in September 1988 (see page 26).

11/16/88

Water at the Interface: Neutron Diffraction Research at Kent

by Henry A. Resing.

Ubiquitous water – 90 percent of our physical being, principal component of our nourishment, determinant of the climate, medium of growth, medium of corrosion and decay – remains yet in many senses mysterious, especially with regard to its molecular interaction with surfaces. And such surface interaction is functionally very important: water filtration in kidneys, spoilage of frozen food, nucleation of rain, aggregation of proteins, hydration of metal ions (to merely start an enumeration).

At the University of Kent (Canterbury, UK) there is considerable concentration on the properties of solids and liquids in their finely divided states. J.C. Dore and collaborators at the Physics Laboratory have made structural studies on the freezing of finely divided water, both "free," as obtained from the rapid freezing of droplets produced in supersonic jets, and "interfacial," as contained in the pores of silica gel (mean pore diameter 90 Å).

In the case of the free water, the question was the nature of the amorphous water formed by condensation from the gas at liquid nitrogen temperatures. If a glassy or amorphous state of water could be produced by cooling bulk water through its glass transition, would it be the same as that obtained by condensation? Efforts to cool liquid water through its glass transition have a long history, but it is only by the supersonic jet technique that this could be done reproducibly. Dore's group have recorded neutron diffraction patterns for both sorts of amorphous water and found them to have identical structures. Question answered. That is, it makes no difference with respect to structure whether the amorphous state is produced by adding one molecule at a time or by the "glassification" of a collection of molecules. This is important input data for those who are concerned with the molecular mechanics/dynamics of hydrogen-bonded systems and the computer simulation of same.

In the case of the interfacial water the questions are:

- Does it freeze, e.g., take up an ordered structure as the temperature is lowered?
- If it does, how is that structure related to that of ordinary ice?

By neutron diffraction, Dore's group are finding that there is a gradual freezing transition for the water in the 90-Å pores and that the "ice" formed is cubic rather than the hexagonal ice formed from bulk liquid water. They are seeking to explain all the features of the diffraction pattern in terms of a disordered cubic ice, rich in stack-

ing faults, with an accompanying fraction of amorphous water. New questions arise as to whether the water structure depends on:

- The nature of the surface which bounds it, e.g., polar, hydroxyl bearing, fractal geometry (i.e., roughness, radius of curvature, etc.)
- The degree of filling of the pores
- Temperature

or even

- The mass of the hydrogen species in H_2O.

For these neutron diffraction studies, facilities at the University of Oxford and the Harwell Laboratory in the UK or CERN (Grenoble, France) are used. The water studied is necessarily D_2O.

The next step is to use other structural and dynamical probes of such finely divided matter as nuclear magnetic resonance (NMR) and dielectric relaxation, computational chemistry, etc. Then one must pursue the behavior of molecules which interact with surfaces by means of force laws other than the hydrogen-bond attraction which typifies water. Investigators at the Physics Laboratory at Kent have decided to concentrate on just these areas of condensed matter research. The use there of NMR relaxation to study freezing of cyclohexane in the pores of silica gel was commented on previously in *ESNIB* 88-06:13-14(1988), reported below.

Professor John Strange (head of the Physics Laboratory) and collaborators are extending their NMR work to absorbed alcohols and short chain hydrocarbons – the stuff of catalysis. They are using relaxation techniques which have been available for a long time; despite their availability, such techniques have not been assiduously applied in surface chemistry except in a few laboratories (Leipzig, NRL, Hamburg, MOBIL). These techniques provide rates of molecular diffusion, rotation, and chemical exchange which are rather cheaply, easily, and straightforwardly available. Unfortunately, they are being neglected in the rush to megabuck NMR.

Kent's Professor Jack Powles, one of the world's experts on molecular motions in liquids, is turning his skills to computational simulation of the structure and dynamics of finely divided liquids. Professor A. Chadwick of the Chemistry Laboratory is using NMR to study the effects of crystal size on the conductivity of two-phase solids; an anomolous increase is noted for small ionic crystals mixed with silica gel. I hope to report on these areas in more detail in a future *ESNIB*. But the point here is that a relatively small university has marshalled its resources to concentrate effectively on nano physics and chemistry, the hot topics of the 1990's.

11/16/88

Applications of NMR in Colloid and Interface Science An International Conference

by Henry A. Resing.

This article, written while Dr. Resing was still at the Naval Research Laboratory, was first published in ESNIB 88-06. It is reprinted here to bring together all of Dr. Resing's writing for ONREUR in one document.

Professor Terrence Cosgrove of the University of Bristol, UK, arranged this superb meeting of the British Radiofrequency Spectroscopy Society (5 through 8 April 1988) in Bristol. Of the more than 100 attendees most were from the UK; the largest foreign contingent was from Sweden (about five) with representation from West Germany, France, Belgium, Denmark, Switzerland, the Netherlands, East Germany, and the US. Chemists, physicists, and chemical engineers made up the interdisciplinary group. Cosgrove intends that there be a symposium proceedings, to be included in a regular issue of the journal *Colloid and Surface Chemistry*.

Although zeolite catalysts and lyotropic liquid crystals comprised the two areas of of heavy emphasis, a full range of interfacial phenomena were covered by the conference, as this report reflects. Personally I am ever amazed at the constantly growing power of nuclear magnetic resonance (NMR) spectroscopy in surface chemistry; the power to analyze surface functional groups quantitatively and qualitatively, to measure dimensions of surface entities, to find the orientations of adsorbed molecules, to measure the kinetics of surface reactions, the power to say when microscopic regions are connected or

not connected, and so on ad infinitum! Read on for but a sample.

Catalytic Surfaces

A first highlight of the meeting was the lecture by H. Pfeifer (Department of Physics, University of Leipzig, East Germany). His group has masterfully defined the state of the art for high-resolution proton magnetic resonance in the solid state, and in the process they have completely elucidated the acidic groups of the available rouge of zeolite cracking catalysts. Such catalysts are now the mainstay of the petroleum industry for cracking and reforming processes; the rate of the cracking process depends on the concentration of a certain one out of five types of acid groups Pfeifer's team has identified. Pfeifer and coworkers were able to use the spin-counting property of NMR spectroscopy (i.e., for any proton-containing functional group in the sample the signal intensity of its resolved line is proportional to its concentration) to measure the concentration of the crucial bridging hydroxyl group of the large cavities.

To do this, Pfeifer's group first had to resolve the proton NMR lines of the expected five groups, namely, of the (a) silanol, (b) extra-frame-work aluminate, (c) large cage Al-(OH)-Si bridging, (d) small cage bridging, and (e) ammonium groups. This involved the design and construction of "magic angle" spinning chambers in which each of the hundreds of zeolite specimens could be sealed under vacuum. No other laboratory in the world is able to do this on such a routine basis: this was technical advance number one. Second, these researchers had to identify the NMR lines. This was done by a careful correlation of the NMR spectra with infrared spectra in the light of what was known about the histories of the zeolite samples (e.g., type, exchange degree, heat treatment, etc.). Third, they had to identify the functional group (and its NMR line) that affected the cracking efficiency; it is the bridging hydroxyl in the large cages. Fourth, having found the responsible functional group they were able to correlate its catalytic effectiveness with the theoretical electronegativity of the zeolite lattice as a function of Si/Al ratio. The Si/Al ratio is the fundamental composition variable in zeolite science – i.e., it is under the industrial chemist's control, and, as a result, catalytic efficiency is also under his control.

The lecture and the research on which it was based were both tours de force and deserve greater exposure and acclaim than they are getting. No one from the Leipzig group has ever spoken in the US, although plans are under way to bring Pfeifer to the US for the Fifth International Symposium on Magnetic Resources in Colloid and Interface Science to take place in Delaware in 1989 – university and industrial laboratories please take note. (Write to: Professor Cecil Dybowski, Department of Chemistry, University of Delaware, Newark, Delaware 19716.)

J. Klinowski of the University of Cambridge, UK, reported that he was able to determine the molecular dimensions of this highly important aluminate bridge hydroxyl group. He reported also on his use of ^{29}Si NMR as a tool to measure the Si/Al ratio in zeolites.

B. Boddenberg (University of Dortmund, West Germany) has been able to find the orientation of molecules with respect to highly graphitized carbon surfaces, even if he used powdered samples. He notes (theoretically) the effect of the magnetic susceptibility on calculated powder NMR spectra: the known orientation of the susceptibility tensor with respect to the surface of graphite gives the index of surface orientation – a neat trick.

J.H. Strange (University of Kent, UK) reported on his study of the isothermal crystallization of cyclohexane enclosed with 90-Å pores of silica gel. He observed that freezing points were depressed, but the thermal and dynamical properties of the molecules proved similar to the bulk. He, along with T. Cosgrove (University of Bristol, UK), used quasi-elastic neutron scattering techniques – at the European Center for Nuclear Research (CERN) in Grenoble, France – in conjunction with NMR techniques. Said Cosgrove of their works on this project in France, "It's such a dream to go to CERN-Grenoble; everything works perfectly. All one has to do is bring the samples." (However, he added, very detailed planning is required in order to be productive.)

This "switch" to nuclear scattering is driven not purely by a desire to enhance scientific understanding, but, at least in some measure, is due to the unavailability of new magnetic resonance facilities for academic departments in Britain. For instance, Professor J. Luckhurst (University of Southampton, UK) mentioned that only $1.9 million are available for capital spending on university chemistry in the UK this fiscal year. On the other hand, the costs at Grenoble come from international agreements as well as from other pockets.

Cosgrove was able to achieve complementary results from both techniques from polyethylene oxide adsorbed from solution onto spherical silicon particles. Binding coefficients as well as mass distributions as a function of distance from the surface were revealed.

Liquid Crystals

The second highlight of the meeting was the review by G. Lindman (University of Lund, Sweden) on oil/water microemulsions. In certain of these systems, stabilized by adding surfactants, one is able to go smoothly from a condition in which water is dispersed in oil to one in which oil is dispersed in water. This is revealed by the fact that when the water is dispersed – i.e., locked in micelles – it diffuses slowly, but when it encloses the oil in micelles it

diffuses as freely as in the normal liquid. How this can happen without a phase change is quite mysterious, but happen it does. Lindman presented diffusion data for several systems; this data was obtained by the now familiar pulsed gradient NMR technique. The data require that at low water content only the oil-rich regions are connected but that at high water content only the water-rich regions are connected. At intermediate concentrations there is the bi-continuous region for which both the aqueous and oil phases appear to be connected. Lindman suggested a layer structure that would allow this. However, O. Soderman (also from Lund University) suggested that there were, instead, very unstable situations which went from one connectivity to the other quite rapidly. Lindman also discussed the NMR evidence for multiply connected cubic liquid crystalline phases.

N. Boden (University of Leeds, UK) presented a set of order parameters for liquid crystals composed of discotic micelles. S. Zumer (University of Ljubljana, Yugoslavia) discussed work he had begun at the liquid Crystal Institute in Kent, Ohio, on liquid crystal globules dispersed in polymers; here the goal was the practical one of making an optical switch. For small dispersed globules, order was imposed by the interface of the polymer with the globule, and was not "switchable." This was in contrast to switchable, larger globules.

Thus the meeting touched on solid-gas, solid-liquid, solid-solid, liquid-gas, and liquid-liquid interfaces. Quite a success!

5/9/88

Zeolite Catalysts at the Imperial College of the University of London

by Henry A. Resing.

Zeolite catalysts began their transition from laboratory curiosities to magic wands of industrial chemistry under the direction of Professor Richard M. Barrer of the University of London's Imperial College of Science and Technology. When he found them, zeolites were merely a strange class of naturally occurring hydrated minerals which had the curious property that they could lose water on heating and yet retain their original crystal structure; the erstwhile water sites are then replaced by a network of pores. Barrer oversaw the transition of porous zeolites to useful "molecular sieves" by which molecules could be separated according to size; he devised methods of synthesizing them in the laboratory and discovered new zeolite species unknown in mineralogy; he studied exchange of the intracrystaline ions – on the one hand to scavenge calcium ions from hard water and, on the other hand, to introduce catalytically active "sites" such as hydroxyl bridges (see *ESNIB* 06-88:13-14[1988], reported above) or paramagnetic ions into the pores. Barrer's "beginnings" have led to methods of industrial chemical synthesis, based on zeolite catalysts, which dominate the modern scene, especially with respect to the production of gasoline; and led as well to the phosphateless detergents of today. His work thus touches all of us in the industrialized world, and with such positive impact that it is surely Nobel-prize worthy. Professor Lovat V. C. Rees believes this, and so do I. Barrer, in his eighties, continues as emeritus professor at Imperial.

Professor Rees (Imperial College, Department of Physical Chemistry) continues work in that department on the chemistry of zeolites. In addition, he is a principal for the UK in the assessment of safety factors for the disposal of nuclear wastes. Both of these efforts involve studies of rates of diffusion in solid materials: molecular diffusion in zeolite crystals and catalytic beds, and ionic diffusion in clay beds or ocean sediments for the nuclear wastes.

Separation of gaseous mixtures of small molecules by pressure swing adsorption over zeolitic adsorbent beds is the current method of choice for the *in situ* generation of oxygen from air (hospitals, home units) and nitrogen (shipment of agricultural products). Rees is concerned with use of the method for separation of petrochemical mixtures (e.g., of methane, carbon dioxide, hydrogen, etc.). Thus his group studies multicomponent gas equilibria over zeolite adsorbents. They have found it practical to study adsorption on a large mass of crystals which practically fill the adsorption volume; a two-component gas mixture of known composition and mass is then introduced into the volume and allowed to equilibrate at a given temperature, after which the pressure is read and a small sample of the gas is withdrawn for analysis by mass spectroscopy; the sampling is repeated at various temperatures, and the whole process repeated for various compositions and masses of gases. The nicety of the method lies in the fact that the composition in the ad-

sorbed state is always known; it is the chosen composition of gas introduced. The method works well at high pressures.

Pressure-swing separation methods are more economical in energy than the standard separation procedure of distillation, but change to them on an industrial scale is not favored by the current low price of petroleum feed stocks. In zeolitic pressure-swing separation processes as well as in industrial reaction processes over zeolite catalysts, the rate of molecular diffusion as a function of molecular mass and shape is a determinant of success.

For a long time there has been a discrepancy between different methods of measuring diffusion coefficients within the pores or channels of zeolite crystals. Nuclear magnetic resonance (NMR) methods, which are carried out at equilibrium, have given diffusion coefficients about a hundred times greater than those provided by the more traditional "rate of equilibration" methods. Proponents of both methods stoutly defended their techniques. The discrepancy could have nothing to do with imperfections in the macroscopic structure of the zeolite crystals; both methods purported to measure the same process. Rees' group have recently shown that when zeolite crystals are held in isolation from one another and their rate of equilibration is followed, the same diffusion coefficient as for the NMR method is found. Somehow, the packing of the crystals together prevents them from following the law of equilibration that one would predict on the basis of the crystal shapes and Fiock's laws of diffusion. To study such equilibration rates Rees and his coworkers have constructed a volume-jump cell in which the volume enclosing the gas and adsorbent is modulated by a square wave; the pressure oscillation and its phase relation to the volume oscillation are then measured. Fiock's laws do the rest. At present they study ZSM-5 zeolites.

Under industrial conditions hydrocarbons degenerate rapidly on zeolite catalysts into coke, which clogs the channels, and a regeneration step is then required. It has been found that if the aluminum content of Y zeolites is adjusted to 32 atoms per unit cell (from the normal 56 atoms per unit cell) the lifetime between regenerations is optimized. Rees et al. are finding that this adjustment can be made, at least on a laboratory scale, by refluxing Na-Y zeolite with $SiCl_4$ in a suitable solvent; silicon replaces aluminum in the framework. They are seeking to extend such simple procedures to the removal of extra-framework aluminum from Y zeolites, as well as to the insertion of iron or titanium into the lattice of ZSM-5 zeolites. Similar studies are under way to improve the binding properties of A-zeolites for magnesium in water-softening (detergent) applications. They have installed a new computer-controlled x-ray powder diffractometer to assist in this work.

Rees has been concerned with the binding properties of radioactive actinide ions in clays and with the functional groups of humic acids in clays and in ocean sediments. He has specifically studied neptunium. His conclusion is that the equilibrium constant so strongly favors the binding of actinides to the huniec acids that those ions are effectively immobile with respect to long-range transport – into aquifers, in the case of land-based storage facilities, or out of the sediment of the ocean floor in the case of possible ocean floor disposal (the latter he sees as quite unlikely due to international ramifications). His next step is the evaluation of actinide binding by "pure" clays – i.e., clays free of organic residues.

As an aside, Rees commented that the Physical Chemistry group at Imperial College were marching together toward retirement, and that steps toward renewal need to be taken. They have decided to handle the situation by preparing to turn over each individual research group to a "successor in training." Such apprentice group leaders are now being sought.

12/14/88

Chemical Structures via Neutrons and X-rays in the UK

by Henry A. Resing.

"New Radiation Sources for Chemical Crystallography" was the topic of a 1-day meeting of the British Crystallographic Association held at Birkbeck College, London, on 16 November 1988. The neutron source is at the Rutherford Appleton Laboratory near Cambridge. X-rays are provided at the Daresburg synchrotron facility operated by the the Science and Engineering Research Council (SERC).

Dr. C.C. Wilson of Rutherford emphasized that production of neutrons by the splitting of uranium via a

pulsed proton beam gives a time reference to the neutron beam. As there is a broad range of neutron energies, the time reference allows them to be sorted by time of flight (TOF); the diffraction condition $\lambda = 2d \sin \theta$ is thus met at fixed orientation θ of the detector by using the range of λ available. Such fixed-detector orientation should be extremely useful in high-pressure experiments where only certain detector-beam orientations are favorable. This single orientation-TOF method is appropriate to powder diffraction experiments, as is the high-angle backscattering method, with a high-resolution, position-sensitive detector. The latter method is being used to refine and determine the effect of thermodynamic phase changes on the position of hydrogen atoms (e.g., squaric acid, malonic acid), where difference projections prove useful. When the detector for single crystal diffraction is developed, it is anticipated that data acquisition for protein crystals 0.1 mm on a side will take only 45 minutes and that for larger crystals "real time" (1 s) structural changes will be resolvable.

Four lectures on the synchrotron x-ray source at the SERC Daresbury Laboratory followed. Dr. A.M. Glazer (University of Oxford) pointed out that it was important to use this expensive source only for experiments which could make use of its unique attributes: parallel x-ray beams; white radiation; polarization in the plane of the storage ring orbit; time resolution through bunching of electrons; and high flux intensity. The time resolution and broad energy spectrum provides again the time-of-flight/single-detector orientation advantage as for the neutrons. It turns out that many crystals for which the reflection-peak (solid-angle) width is determined by crystal perfection can be done as well on conventional x-ray apparatus. The flux intensity gives rapid signal acquisition; the flux intensity will be 10^5 times higher at the European Synchrotron Radiation Facility now under construction at CERN, and it is not known at present how these fluxes will be detected and otherwise handled. The broad range of energies allows beam energies to be chosen around the absorption edges of certain heavier elements.

Margaret Harding (University of Liverpool) emphasized the application to small crystals of difficult-to-crystallize materials as an example of proper use of high flux density. In general, the diffraction spots of such crystals show streaks in at least one dimension (5-6° mosaic spread), which indicates that there is an intrinsic disorder which actually prevents the growth of large crystals. Another example was the reaction of a crystalline protein with a substrate as followed *in situ*. The unit cell dimensions remained the same while the substrate was incorporated, and the location of the substrate could be found by differences in the projections before and after reaction. Harding estimates that adequate diffraction data may be obtained from more perfect crystals as small as $5\ \mu^3$.

Anomalous x-ray scattering (AXS), which depends like EXAFS on spectrometry about the absorption edge of a given element, but which has a somewhat longer range, was discussed by A.G. Orphen (Daresbury). As an example, for $NiCL_2$ in 4.2-molal aqueous solution, Orphen showed that the first coordination sphere for Ni contains, to good approximation, only H_2O (EXAFS of Ni) while the second coordination sphere holds the Cl ions (AXS of Ni). EXAFS of the chlorine showed at most one-third of a Cl^- in the first coordination sphere of Ni^{++}.

S. Bailey (Daresbury) and collaborators used the differences in x-ray scattering with frequency about the absorption edge of iron to force different projections and to find the two different iron atoms in certain poorly crystallized two-lobed transferin molecules. For the rest of the molecule, only 3-Å resolution could be obtained.

The thrust of the meeting was a desire by those who are developing the new spectroscopies – about 70 percent, physicists at the Rutherford Laboratory say – to hand over these tools to scientists whose interest would be in the systems studied and the advantages the tool would give them rather than in the techniques themselves

12/14/88

Functional Fluids at the Royal Holloway and Bedford New College of the University of London

by Henry A. Resing.

Professors D.G. Gillies and L.H. Sutcliffe have pooled their resources and expertise to form what they have named the "Functional Fluids Group." It is located in the Chemistry Department of the Royal Holloway and Bedford New College (RHBNC) of the University of London. RHBNC is a college of some 3000 students – the

only college of the university not inside the city limits of London (it is in Egham, Surrey), and which is projected to increase in resources as a center of instruction in the sciences.

As a center for the sciences, the Functional Fluids Group has captured the university's new multinuclear solid-state nuclear magnetic resonance (NMR) spectrometer. This instrument sees 24-hour-a-day service, only one-fourth of which is devoted to work on functional fluids, with the remainder used under the "intercollegiate research service" for research by other colleges and other groups of the university.

The Group benefits greatly from being part of the university's intercollegiate service because many instruments of other colleges are shared. Limiting consideration to NMR facilities of the University of London, I note that University College, London, shares a 500-MHz (proton) liquid-state spectrometer, Queen Mary College a 400-MHz, and Kings College a 250-MHz, with still other lower frequency spectrometers at RHBNC. A novel feature of this collegiate approach is that when a student at one college needs a facility at another (say some 20 miles and $10 away) the out-of-pocket expense he incurs is borne by the university system. This broad frequency capability in high-resolution C-13 NMR provides a unique tool for application to the set of functional fluids:

- Lubricants
- Surfactant solutions
- Electrorheological fluids
- Fuels.

As part of an effort in Britain to share research costs with industry, the RHBNC group has attracted support for what is termed "pre-commercial" research from British Petroleum, Castrol, and Shell for research projects, which are essentially basic in character. This success in funding has prompted the Scientific and Engineering Research Council (SERC) to look at "functional fluids" as a separate research category at a meeting which took place last December.

Gillies contends that the time is ripe for a detailed look at the molecular motion of lubricants currently in use or of potential use. High-resolution NMR allows spectral lines for each functional group of a hydrocarbon molecule to be resolved, and the relaxation time of that group to be measured. The frequency dependence of the relaxation time – available by means of that grand suite of spectrometers – allows certain autocorrelation functions of relative interatomic positions to be deduced. His group has examined the following suite of molecules (each in some sense a model of a typical lubricant):

- Octyl chloride
- di-m-octylether and
- tri-m-octylamine

The Group has characterized them all (according to their first look at the data) in terms of two independent molecular motions, the time scales for the two motions being different by orders of magnitude. The Group plans to follow the pressure dependence of the NMR relaxation (at high resolution) up to about 10 kbar, a type of work of which few laboratories in the world are capable. The Group's researchers find that such high-pressure work, which involves construction and design of suitable apparatus, is only possible because they have associated with them an extremely capable machinist who can fabricate and assist in the design of the vessels, seals, transducers, etc. They are aiming for computer control of temperature and pressure in a programed set of high-pressure experiments.

With respect to these lubricant systems, Sutcliffe intends to do electron-spin resonance spectroscopy of small, free radical probe molecules therein, to further elucidate molecular motions. He plans to use infrared and Raman spectroscopies, as appropriate, on these systems and to simulate results via Dr. David Heyes' molecular mechanics by calculations. The ultimate aim, of course, is to correlate molecular motional results with lubricant properties and thereby provide some feedback into lubricant design. This is obviously a long-range plan, but one which would be worthy of any US Navy laboratory.

Another part of the RHBNC program – electrorheological fluids – was something new to me but something known in the literature for 50 years. Certain two-component systems (i.e., solid dispersed in liquid) congeal or stiffen in an electric field even though they are quite fluid in the absence of a field. This is a potentially useful mechanical clutch device. The basic science is not yet understood. Evidently many different solid/liquid pairs show such behavior. RHBNC student P. Bailey has found that certain kinds of zeolite crystals (porous hydrates) do or do not show the stiffening, depending on the amount of water or upon the counter-ion species present within them. He is attempting to understand this through magnetic resonance studies of the water, the ions, and of free radical probes in the interior of these zeolites. This is all part of the question "Does the conductivity of the dispersed solid have anything to do with the mechanism of stiffening in the electric field?" Evidently, too high a conductivity kills the effect, but solids of roughly the same conductivity and with similar crystal structures show wide ranges of stiffening behavior. An adventurous thesis project!

My inquiries as to several other parts of the Group's program brought the answer, "We can't talk about them until the patent claims are filed" – the price one must pay for industrial support.

11/5/88

AERONAUTICS

Aerodynamic Research in Braunschweig, West Germany

by Daniel J. Collins. Dr. Collins was the Liaison Scientist for Aeronautics in Europe and the Middle East for the Office of Naval Research European Office. He has returned to the Naval Postgraduate School where he is a Professor of Aeronautical Engineering.

Two research organizations important in the German aerospace activity are located in Braunschweig, West Germany. One of the organizations is the Technical University Carolo-Wilhelmina and the other is a research center of the German Aerospace Research Establishment (DFVLR). Since there is a close and productive interaction between the two organizations it is appropriate to review their research in the same article. I shall begin the review with a discussion of the Technical University.

Technical University Carolo-Whilhelmina at Braunschweig

Founded in 1745, the Technical University at Braunschweig has the distinction of being the oldest technical university in Germany. One of its distinquished students and later professor was Carl Friedrich Gauss. The university now has 15,000 students, about 300 professors, and around 1300 research associates. As is the case with other German universities the research is organized along institute lines with each institute directed by one or more professors. This university has about 120 institutes and of these institutes my primary interest was in the Institute for Flight Mechanics and the Institute for Flight Guidance and Control. In the course of my visit I was informed of an interesting interdisciplinary research organization called the Center for Air and Space Technology (ZLR), which merits a brief discussion.

ZLR is a university-recognized center founded in 1987 by 10 professors from eight independent institutes. In addition to the institutes mentioned above there are the institutes of fluid mechanics, aircraft design and structural mechanics, space engineering and nuclear engineering, internal combustion and jet engines, traffic engineering, and control theory. What I find interesting about ZLR is that it duplicates what in America would be called a department. The essential idea is that larger projects can be undertaken by the center than would be the case for the smaller institutes, which have typically one professor – although often with many associates. German professors function like medieval barons in their own institutes and it would be worthwhile, in the future, to see how what I have called the American departmental structure fits in with the German institute structure. I shall now turn to a discussion of the two institutes that I visited.

Institute for Flight Mechanics. Professor G. Reichert directs the Institute for Flight Mechanics, which has 15 research and teaching associates nearly all of whom are working for their doctoral degree. Reichert had extensive experience in the German helicopter industry before becoming the director in 1983. Ten of the associates are supported on research projects which are funded by the German Ministry of Research and Technology (BMFT) and the German Society for the Advancement of Scientific Research (DFG). The two research directions of the institute are connected to the flight mechanics and dynamics of rotary-wing aircraft and to the flight mechanics of fixed-wing aircraft. For fixed-wing aircraft the emphasis is or the impact and potential of active control technology and the influence of new configuration such as canards. The current main effort in the research program of the institute is, however, on rotary aircraft.

For rotary aircraft, or helicopters, the emphasis is on improved mathematical models and calculation methods, on flight measurement techniques, and on flight safety procedures in takeoff and landing. Much of this work is in cooperation with DFVLR at Braunschweig, which thus also involves technical exchanges with the United States. As part of the program with DFVLR the institute is constructing a model helicopter with a 1.5-meter rotary blade diameter which will be tested in the 3-meter low-speed tunnel at DFVLR. The model is to be used as a test bed to verify theoretical calculations and stability studies. Full flight-test comparisons with theory and data reduction methods are currently being studied in a joint project with Messerschmitt-Bölkow-Blohm (MBB), Universität der Bundeswehr, DFVLR, and Henschel-Flugzeugwerke. The helicopter model may help in understanding discrepancies (Liese et al., 1987).

Extensive studies and tests have been made on the BO 105 helicopter in takeoff and landing tests. The prob-

lem is reasonably complex and can involve ground resonances and autorotation of the blades in the case of engine failure. These studies have also included other helicopter configurations such as those with multiple engines and different rotor modeling – for example, articulated and fixed rotor blades (Cerbe and Reichert, 1987).

Institute for Flight Guidance and Control. The Institute for Flight Guidance and Control, which has some 40 research associates, is subdivided into two main parts: Flight Guidance and Flight Control. Flight Guidance is led by Professor G. Schanzer, Flight Control by Professor R. Brockhaus. The main research directions are in flight experiment and measurement techniques, flight meteorology, position finding and navigation, man/machine interfaces, flight simulation, and flight and engine control. Supporting the institutes' research objectives are two aircraft, both are two-motored (one is a Dornier DO 128), and a research flight simulator. The institute has many projects supported in part by DFG, BMFT, ESA, BMV, the Fraunhofer Gesellschaft, and industry. I shall mention only a few of what I considered the more interesting projects.

One of the main research projects of the institute is connected with a national effort on aircraft safety in the flight region close to an airport. This project is interdisciplinary and is concerned among others with takeoff and landing and with estimation of flight variables (Brockhaus). The takeoff and landing investigation is concerned with variable wind surface conditions such as wind shear and wing tip vortices generated by large aircraft. The project is directed by Schanzer with coordination by Brockhaus. Some of the other areas of investigation include meteorology of the atmospheric boundary layer, collision avoidance, air traffic control, and data security. The University of Berlin, the University of Hannover, and DFVLR are involved in this long-term project, sponsored by DFG, which has already lasted 6 years.

Another problem under investigation in the Flight Guidance area is peculiar to the Stuttgart airport. The landing approach at Stuttgart passes by the Weidacher mountain, which generates large wind loads on the aircraft. The effect of these winds are being analyzed with a view to improving the safe landing capability of the airport. Finally in this area, there is what I would term a fun project – investigating the energy transfer between wind and glider aircraft. The Germans have had a tradition of excellence in research on gliders but I would have expected this work to be in a fluid mechanics institute rather than in a flight guidance and control institute.

Most of the projects in the flight control area are funded by DFG. The work on identification and system parameter estimation is based on nonlinear observers and, further, involves analytical redundancy so that the input data to the pilot and the flight controller is more reliable and therefore safer. A recent application of this approach has been to the second airplane used in the flight program of the institute, the Dornier DO 28. A nonlinear multipoint model of the Dornier DO 28 was developed for the longitudinal motion of the aircraft. Finally, I want to mention that new linear and nonlinear controller structures are being developed for aircraft engines.

German Aerospace Research Establishment at Braunschweig

The research center of the German Aerospace Research Establishment (DFVLR) at Braunschweig has it origins in an aeronautics laboratory established by a professor of the Technical University at Braunschweig in 1931. Undoubtedly for this reason, at least in large part, there has been a strong tradition of cooperation between the two institutions since then. DFVLR is a large organization with five research centers which, in addition to the one located at Braunschweig, include those at Göttingen, Koeln-Porz, Stuttgart, and Oberpfaffenhofen. The Braunschweig center's scientific staff is divided into five research departments and three supporting departments with a total of about 2500 personnel. The departmental structure can be composed of elements from different centers as is the case for the department in which I had a particular interest – the Research Department for Flight Mechanics/Guidance and Control. There are four institutes in the department, two of which are located at Braunschweig, one at Koeln-Porz, and one at Oberpfaffenhofen. I have already reported on the work of the Institute for Flight Systems Dynamics at Oberpfaffenhofen which is under the direction of Dr. J. Ackermann (*ESNIB* 88-03:45-47[1988]). The institute at Koeln-Porz is concerned with aerospace medicine.

Braunschweig has the Institute for Flight Mechanics and the Institute for Flight Guidance. I should mention that the word "institute" has been taken over from the German university context but the DFVLR institute can be much larger than an institute in a typical university. Thus the Institute for Flight Mechanics, directed by Dr. P. Hamel has over 130 people – about half of whom are scientific personnel. Although the primary focus of my visit was the Institute of Flight Mechanics, I would like to list the research areas of the Institute of Flight Guidance, these include telemetry and flight data systems, navigation, measurement techniques and sensors, and human engineering. Some of the facilities of the institute include a research flight simulator with a four-degree-of-freedom motion and an air traffic control simulator.

Institute for Flight Mechanics. I was fortunate enough to attend a short German workshop or study course (Flight and System Simulation) given by the Institute for Flight Mechanics. Since a substantial part of the course was given by DFVLR personnel (with detailed

discussion of computer methods and techniques and with in-depth visits to simulation and aircraft facilities) I gained, perhaps, a better understanding of the work conducted at the Institute of Flight Mechanics than would have been possible in a short visit of a day or two. Dr. Hamel was also most helpful in his discussion with me on the work of the institute.

The research activities of the institute can be categorized into five main areas: flight mechanics of aircraft, flight mechanics of helicopters, real-time and in-flight simulation, mathematical methods and data handling, and flight test instrumentation. I would like to highlight the first three sections but I will make some briefer remarks on mathematical methods and flight test instrumentation sections.

Flight Mechanics of Aircraft. The section called flight mechanics of aircraft is strong in the area of identification and determination of the dynamic parameters of an aircraft. Although determination of the static parameters of an aircraft can normally be determined relatively easily, the determination of the dynamic parameters of an aircraft is a difficult task. The section has the capability of dynamic simulation in a wind tunnel using oscillation of the model, free-flight testing of a full aircraft, and, in a cooperative program with the Institute for Fluid Mechanics of Lille in France (IMFL—see *ESN* 41-9:510-512[1987]), of free-flight testing of models. Previous experience in gust alleviation and the modeling of nonlinear nonsteady effects in gusts and rapid motion of control surfaces is now being applied to the identification of unsteady aerodynamic effects on the X-31 aircraft for the US. In this respect there are several memorandums of understanding for exchange of technical data between DFVLR and various agencies of the US Government.

Flight Mechanics of Helicopters. Somewhat similar activities are conducted by the flight mechanics of helicopters section in that identification and parameter estimation is an important research area. I have already indicated the system identification work on the BO 105 helicopter in my discussion given above of research at the Technical University. The identification algorithm is based on the maximum-likelihood method in the time domain. Included on the modeling is the effect of the higher frequency rotor dynamics, which can have a significant effect on the response of the helicopter. A long-duration experimental program (over 5 years) in the large German-Dutch wind tunnel (DNW) has been directed at dynamic rotor tests of the BO 105 rotor, which is manufactured by MBB. Active control techniques were developed for the test stand in order to control higher harmonics in the vibration of the rotor. Hamel indicated that the institute does considerable work in the DNW facility which is particularly directed at noise abatement.

Both the aircraft and the helicopter sections are involved in theoretical work on model-following control systems. One recent report is on an improved design technique for model-following control systems in "In-Flight simulation" (Henschel and Chetty, 1987). New measures based on the singular value decomposition resulted in lower and more practical gains with respect to earlier designs and with increased robustness to sensor failure. In a cooperative program with the NASA research center at Ames a robust digital model-follower controller has been developed for helicopters (Bouwer, 1988). The controller structure is independent of the explicit plant model and can be used with different plants. This is a useful feature since the characteristic parameters of a helicopter are generally not known exactly. A recent report to the August 1988 ICAS meeting in Jerusalem by both Henschel and Bouwer reports on the application of the model-following control system for both fixed-wing and helicopter aircraft. The feedforward gains are calculated using the pseudo inverse of the control matrix while the feedback gains are based on an interactive vector performance optimization technique.

Real-Time and In-Flight Simulation. A major effort of the institute is in the area of real-time and in-flight simulation. The DFVLR's new flight test aircraft, which is called ATTAS (Advanced Technologies Testing Aircraft System), is a two-jet aircraft based on the VFW 614, the first civil airliner built in the Federal Republic of Germany. ATTAS is used to test concepts in integrated digital control systems, in air traffic control, in in-flight simulation, and in wing aerodynamics. The emphasis in the real-time and flight simulation section is naturally on the simulation capability of the aircraft. As a flying simulator it is possible to program ATTAS as a jumbo jet or as a new aircraft configuration which needs to be tested. A complete specially developed ground simulator complements ATTAS. The ground facility permits the simulation of flight test of ATTAS in order to ensure safety and to discover problems early in the test program.

Since an actual flight of the test aircraft (ATTAS) is being monitored in any flight program the emphasis placed on real-time simulation of the aircraft is understandable. Special attention is given to the algorithms in the simulation in order to ensure real-time simulation. Special parallel processing hardware, which currently includes an AD10 (manufactured in the US), is also used. The newer machine, the AD100, which greatly enlarges the capability of the system, is now being phased into the hardware configuration. The real-time simulation has recently been expanded to include a BO 105 helicopter so that in-flight simulation with variable stability derivatives can now be done for both fixed- and rotary-wing aircraft. In the helicopter, space considerations preclude the large onboard computer capacity of the ATTAS and more reliance is made on telemetry of the data to the ground simulation facility.

Supporting Sections. The mathematical methods and data handling section gives significant support to the system identification, which is a central research topic at the institute. Identification methods have been developed both in the time and frequency domains. A Cray 1S is used for the calculations involving the identification algorithms. Present work is directed at nonlinear identification, consideration of process noise, and modeling of dead bands and hysteresis. The flight test instrumentation section is concerned with supporting the test technology concepts developed by the Institute of Flight Mechanics. Thus one of the emphases is on development methods for parallel processing in distributed microcomputer systems of high data rates.

Conclusions

The very active program in aeronautics at the Technical University at Braunschweig is mainly of an applied nature, done in close contact with industry and DFVLR. Two of the directors of the institutes that I visited have had extensive industrial experience, which may explain to some extent the applied research emphasis. Important problems in analysis of helicopters are being investigated. Aviation safety in which we all have an interest is another important and wide ranging area of investigation.

The Institute of Flight Mechanics shows great strength in dynamic system and parameter identification methods. The ATTAS project is an exciting technical program which forces real-time simulation which in and of itself is an important technical area. Some very practical advances have been made at the institute in model-following systems for both fixed- and rotary-wing aircraft. There appear to be several important contacts with American research institutions. Finally, the close collaboration of DFVLR with the Technical University at Braunschweig is in my opinion mutually beneficial.

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12/5/88

Aeronautical Research at the Technion

by Daniel J. Collins.

The Technion-Israel Institute of Technology has been for over 60 years a center of technological research in Israel. Over 75 percent of the Israel's scientists and engineers have been trained at the Technion. Each year over 1200 students graduate from the Technion of whom some 70 are doctoral students. Studies are in fluid mechanics and controls concentrated in the Aeronautical Research Center, where the major departmental laboratories are located. The Department of Aeronautical Engineering was established in 1954 and now has 350 undergraduate students and 120 graduate students. About one-third of the research support comes from overseas contracts, a considerable amount of which is from America.

I have structured this article around the laboratories at the Aeronautical Research Center since this is the focus for research. My discussion of the research in the laboratories will concentrate on the research effort of the professors with whom I talked but also included other material which will give some idea of the research directions that I did not have time to cover in my visit.

There are five major research laboratories, the first of which is subdivided into four facilities, which are also called laboratories. The individual laboratories are dedicated to (and named for) study of:

- The Aerodynamics with separate laboratories:
  Wind Tunnel Laboratory
  Aerothermodynamics Laboratory
  Turbulence Research Laboratory
  Shock Tube and Laser Laboratory
- Combustion and propulsion
- Flight control
- Aircraft structures
- Turbo and jet engines

I visited all the laboratories except the one concerned with structures (the Krumbein Aircraft Structures Laboratory).

Aerodynamics Laboratory

The aerodynamic laboratory, which was established in 1956 and now supports 16 senior investigators and about 30 students, has two directions to its research: configuration-oriented aerodynamics and basic fluid mechanics. In the first area work is mainly on modern fighter configurations at high angle of attack with a resulting three-dimensional vortex structure, but recent cancellation of the Israeli fighter has had some impact on the research done in the laboratory. One fascinating subject of investigation has been the aerodynamics of birds of prey.

Professor D. Weihs, who is head of the department, has research interests in flow stability. He is particularly interested in the stability of liquid jets in armor. This work is somewhat sensitive. In a related topic, Weihs is concerned with industrial sprays such as those used for painting. One of his current projects is directed at aerial spraying by the Canadian government against the spruce bug worm.

In the area of instrumentation development and new applications of measurement techniques, Dr. J. Stricker has had a series of papers on the application of Moire deflectometry to the mapping of weak phase objects. Moire deflectometry is an alternate method to, for example, holographic interferometry for the measurement of density fields in compressible flows or other weak phase objects. There are some special advantages in the application of electronic heterodyne moire deflectometry to such measurements since the output is an electronic signal that is readily adaptable to computer analysis rather than an interferogram which needs to be further reduced (Stricker, 1986). Stricker wishes to extend the method to three dimensions and has had support for his work from NASA.

In a very interesting recent paper Dr. J. Rom has investigated a canard-wing configuration at moderately high angles of attack. A nonlinear vortex lattice method (NLVLM) was used with some success in the prediction of experimental lift coefficient variation with angle of attack since pressure distributions are available from the theory. The flow field of the experimental rolled up interacting vortices of the canard and wing were in very good agreement with predictions by NLVLM. In the theory the vortices follow the streamlines. The experimental variation of the canard deflection angle strongly affected the pitching moment and the lift-to-drag ratio, particularly at cruise conditions (Rom and Gordon, 1988). Further details on the NLVLM is given in an earlier referenced paper and earlier experimental measurements of wing-canard configurations were made by Professors A. Siginer and J. Er-El at the laboratory.

One of Siginer's other areas of research is the study and prediction of vortex structure on spinning missiles and munitions and he has developed computer codes to predict such fluid mechanic flows. Siginer has also reported on the Magnus effect on spinning, transonic, finned missiles. In a series of papers he has further investigated the stability of vortices. (Levitas, Seginer 1987).

Professor M. Wolfshtein's major research interest is in periodic flows in ducts and the atmosphere on which he has conducted extensive hot-wire measurements. A natural extension of hot-wire measurements is their use in the characterization of turbulence. In the case of turbulence, Wolfshtein is interested in two-point correlations. He recently spent a month at the Ames (Iowa) computational center working on turbulent correlations in viscous turbulent flows in variable cross-section curved ducts. Rapid distortions create interesting effects on the turbulent distributions and in recent work on a turbulent contraction flow measurements of the turbulence indicated first the expected decrease in turbulence and then an unexpected increase which Wolfshtein's team is now investigating.

Experimental facilities consist of an open circuit 1x1-m subsonic tunnel, an induction-driven transonic tunnel 40 cm x 50 cm, and two moderate-size blowdown supersonic tunnels. Two other small tunnels are used in high-quality turbulence research, and there are two shock tubes, and an environmental chamber. A flexible computerized measurement system includes a laser Doppler anemometer (LDA).

Combustion and Propulsion Laboratory

Work in the area of the combustion and propulsion laboratory was begun in 1969. Five faculty and about seven students are supported through contracts obtained in the framework of the laboratory. The laboratory is well equipped with a variety of measurement equipment to do research in combustion. The propulsion laboratory's area has a control room and six bunkers. Dr. Y. Levy of the laboratory is primarily concerned with diagnostic measurements on combustion systems. In a contract for the Naval Research Laboratory he has developed an on-axis phase Doppler anemometer for spray diagnostics. The system, with a 98-percent accuracy, measures sprays in a size range from 50 to 500 microns with the minimum detectable size around 30 microns. Levy thinks that with some modifications to the system that the minimum size could be reduced to 5 microns. Due to cost consideration Levy has built his own LDA system.

Further application of LDA techniques have been to two-phase flows in the freebroad of a fluidized bed (Levy, 1986). Two-phase flow measurements are inherently difficult. The LDA system was capable of measuring the velocities of the two phases (gas and particles) and the size of the particles, which ranged from 0.2 to 1.5 mm. The tracking particles for the gas phase were at the micron level. A important discovery in the measurements was a

biasing effect that shifts the velocity histograms to lower speeds.

Other work in the laboratory included some space-related work with microgravity combustion, and residual fuel burning in upper stages of landing vehicles. The laboratory also has done work in the design and evaluation of solid propellants, and investigation of solid rocket-motor instability. Other work has concerned ramjets and pulsed-jets.

The Flight Control Laboratory

The flight control laboratory, established in 1971, is staffed with three professors and technician support and normally has about six students. The purpose of the laboratory is to carry out experimental and theoretical research in advanced flight-control guidance and navigation. Professor S. Merhav, who established the laboratory is known for his work in the modeling of the human operator in control loops. Some of his recent work has involved the suppression of pilot-induced oscillations by adaptive filtering. Also involved in this work was adaptive noise cancellation since the noise resulted in involuntary human operator motion. Another recent investigation was directed at an adaptive control based on a normalized variable gain least mean square (LMS) filter (Merhav and Mehta, 1987). The primary purpose of this latter research is to achieve robustness to plant-parameter uncertainty and variations. Stability considerations were addressed in a heuristic manner and the use of variable-gain in the gradient algorithm materially reduced the adaptation rate of the LMS. A model noise suppression scheme also improved performance.

The laboratory has both and moving-base and fixed-base simulators, in one of which I had the opportunity of crashing a plane. A dynamic simulator for remotely piloted vehicles is available and a precision test facility for navigation equipment is also available. Image processing capability for reconstruction of noisy and deteriorated images is included in the laboratory and on-line estimation of aircraft motion is possible from airborne observation of terrain texture.

The Turbo and Jet Engine Laboratory

The turbo and jet engine laboratory was started in 1982 by Professor Gal Or. Much of the work is either proprietary or classified since support is from American engine manufacturers or Israeli military sources. Two large current projects are on advanced tactical fighter engine nozzles. Previous work has involved the F-15 and F-16 flight-ignition and flame-blowout envelopes, and, also, combustion research on the F-100, 1120, and newer engines. There is some interesting work on thrust vector control in process.

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12/5/88

COMPUTER SCIENCE

The MARS Project: Building Deterministic Real-Time Systems

by Krithi Ramamritham. Dr. Ramamritham is a Professor of Computer Science in the Department of Computer and Information Science at the University of Massachusetts, Amherst.

Real-time systems are those systems which are expected to have not only correct logical behavior but also correct timing behavior. Systems that control processes in industrial plants, on-board flight avionics systems, space shuttle software, etc., are good examples of real-time computer systems. Real-time systems

have the special characteristic that they are called upon to behave correctly even under peak loads, for example, during emergency situations when numerous alarms are raised. In particular, unless the emergency conditions are handled within specific deadlines, catastrophic results may occur. In the past, the design of real-time systems has been approached almost as if they had no specific timing requirements. Whether or not timing properties were met was determined via complex simulations of "typical" scenarios. If timing properties are not met, parts of the system parameters are fine tuned – for example, process priorities are adjusted, and code optimization may also be resorted to. This approach, being ad hoc, is prone to errors.

Recently, a number of research efforts have been launched to approach real-time system design in a scientific manner, specifically, to deal with logical and timing properties in an integrated fashion. One such effort is the MARS project (MARS: Maintainable Real-Time System), in progress at the Technical University of Vienna, Austria, under the direction of Professor Hermann Kopetz.

MARS is a comprehensive effort exploring all aspects of real-time system development starting from specification of requirements and ending with system implementation. Goals of the project are to design for fault tolerance and maintainability, and to meet timeliness constraints. Since real-time systems function in environments that are typically physically distributed, MARS is focusing on distributed real-time systems.

Fault Tolerance Through Active Redundancy

Fault tolerance is achieved through active redundancy; i.e., through the use of replicated processing. Replicates are assigned to system components that are designed to be fail-silent through the use of self-checking hardware. Since components are fail-silent, when (parts of) a component fails, it stops producing results that other components may be expecting from it. However, since other replicates exist, the needed results will be produced by those that have not failed.

The MARS Architecture: Clusters of Fail-Silent Components

The MARS architecture calls for a system to be made up of clusters of such components. Components within a cluster lie along a multiaccess bus where communications occur via the time division multiple access (TDMA) protocol. This simple protocol works well, especially if all components impose similar communication loads on the bus. More importantly, since components on a bus transmit in a priori assigned slots, it is possible to know when a message will arrive at its destination. This deterministic communications scheme contributes to the determinacy of the system. Intercluster communication can also occur via TDMA but since the current focus of MARS is on processing within a cluster, this aspect has not yet been explored.

Achieving a Global Time Base

The designers of MARS have spent a substantial amount of conceptual and implementation effort on achieving a global time base, a prerequisite for building a distributed real-time system. This time base is realized by synchronizing the clocks on each component through the use of a VLSI Clock Synchronization Unit that exists on each component. Even though clocks can not be completely synchronized, since in reality the skew between clocks is very small (of the order of a few microseconds), for all purposes, the components can be assumed to function synchronously. This assumption goes a long way in easing operating system as well as applications design. Such tight synchronization has been reached before using additional clock-synchronization-lines on the bus. One advantage of the MARS approach is that this tight accuracy is obtained with a standard bus without additional lines. In addition to a continuous time-base, the Clock Synchronization Unit allows the prompt time-stamping of messages.

All information maintained by MARS components have an associated validity time. A piece of information becomes useless once its validity-time expires. Communication among components is via the exchange of "state messages" – messages that contain information maintained by the sending component and needed by the receiving component. The operating system expunges messages which become invalid.

State messages have the following semantics: Each receiving component has exactly one version of a state message. Thus, when one component sends a message to another, the buffer associated with the state message at the receiver end is updated with the new message. Thus, messages arriving from replicates of a task overwrite the message buffer allocated for the state messages that they produce. Since components are assumed to be fail-silent, the first replicate to produce a new version of a state message updates the buffer. The rest have no effect.

Subsystems of a Real-Time System

Real-time applications typically consist of three interrelated subsystems. The first is safety-critical: if any part of this subsystem fails, a catastrophe could result. The second is essential. As more and more parts of this subsystem fail – i.e., do not meet their deadlines – the sys-

tem performance is degraded. The third in nonessential; this level does not contribute to the safety or performance of the system directly. Real-time system design is complicated by the interrelationships among these subsystems that occur in most applications. Further, if a system is designed to function correctly under peak loads, then under normal conditions the utilization of system resources will be extremely poor because at peak loads (i.e., in emergency situations) the environment produces more data, and a faster rate, than in normal circumstances. This implies that more processing occurs and at a higher frequency under worst-case situations. Ideally what is needed is a design wherein all the safety-critical tasks are executed in emergency situations, and as many essential tasks are executed at all times. In such a system, good resource use will result while taking into account the safety and timeliness properties of tasks.

The MARS Approach to Designing the Safety-Critical Subsystem

The design described above will involve dynamic decision making which, while being flexible, may, however, suffer from unpredictable behavior. Hence the designers of MARS have decided to focus on the safety-critical parts of real-time applications. Specifically, their approach calls for the information about the peak loads to be made available: complete specification about the tasks that will be executed, including the computation time and precedence relationships among the various components of a task, the maximum frequency with which data will arrive, and the expected response time from the system – i.e., the acceptable delay in processing the data. Given this information, the tasks are assigned to various components of the clusters such that the system will meet the specifications of the safety-critical parts of the applications. This task assignment and the scheduling of activities within a component (keeping in mind that the TDMA protocol is used) then forms a crucial aspect of an applications development using the MARS approach.

Since the MARS approach calls for application development based on worst-case requirements, any small change in the requirements specification may cause a complete overhaul of the system. While many process control applications rarely face changes once they are installed, the opposite is true of applications such as those relating to the space station, or even the space shuttle software. These are long-lived applications with evolving requirements.

To reduce the amount of overhaul resulting from evolution, the designers of MARS suggest that initially one should not completely populate a cluster (with the maximum number of components allowed). This is to provide for expansion of a cluster with additional components when processing needs warrant such an expansion. Also, in concept, it is possible to replace a component with a cluster without disturbing the interface of the new cluster (the old component) to the rest of the components in the original cluster. Of course, to make this concept a reality, a number of issues such as the adequacy of the communications bandwidth, the allocation and scheduling changes that may result, etc. have to be addressed. This is yet to be done.

Summary

The MARS project has tackled and continues to develop solutions to interrelated problems in designing the safety-critical subsystems of real-time applications. The strength of the project lies in the fact that the participants in the project have not only developed promising solutions but have also tested their efficacy by implementing them on a cluster of MARS components developed at the Technical University of Vienna. The issues that remain to be attacked include the integrated development of all subsystems of a real-time system in such a way that better resource utilization results and the development of techniques that allow the smooth evolution of applications.

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12/2/88

Posie: Design of an Operating System for Concurrent Computation

by J.F. Blackburn. Dr. Blackburn is the London representative of the Commerce Department for Industrial assessment in computer science and telecommunications.

"Posie" is the name of a project at the Department of Computer Science, University of Edinburgh, aimed toward the design of an operating system which provides efficient run-time support for concurrent, process-based computations. The idea was to look at systems where the architecture supported computations with large-grained parallelism, structured as a set of asynchronous processes communicating by message passing.

Efficient computation depends on both the characteristics of the hardware and the computations to be carried out. For efficient computation, the work must be distributed to take advantage of the processing power of the parallel processors – without unduly increasing the communications traffic between processors. Since requirements for computing and for interprocess traffic may not be known until run-time, it may be important to support process migration to balance the processor loads and to move processes which exchange much data closer together. Thus, Rob Pooley and Rosemary Candlin decided to investigate the use of process migration to provide dynamic load balancing (Pooley and Candlin, 1988).

Objectives

Pooley and Candlin's idea is to study the properties of large-grained parallel computations from the theoretical, simulation, and measurement points of view. The aim of the theoretical work is to provide abstract models of important classes of parallel computations. A computation can be described at a number of different levels of detail, which must be consistent. However, different levels of detail may be appropriate for different purposes. A model can be described by a formal specification which makes clear what assumptions have gone into the model, and to what constraints it is subject.

Simulation allows study of the effects of different strategies of process placement and migration for different machine topologies and computations. The plan is to build a set of modeling tools to experiment with these factors, and to identify sensitive parameters. There will be an interaction with the theoretical work in that the simulation models will be described formally. Also the simulation may cause changes in the theoretical models.

One reason for learning about the statistical properties of real parallel programs is that any operating system must be tuned to handle the kind of programs most likely to run on it. Also, statistical distributions of system parameters are required as inputs to the simulation models. Real-time data on processor loads and bus traffic are needed to enable decisions about process migration and rerouting message traffic.

In order to get measurement information without altering the results of the computation or seriously degrading system performance, a decision was made to construct a machine with built-in monitoring facilities.

Work in Progress

Theoretical Basis. Pooley and Candlin's initial intention was to build descriptions of the systems in Robin Milner's Calculus of Communicating Systems and to demonstrate their properties. They found, however, that they needed a less ambitious, more abstract model of concurrent computation as a means of defining notions such as "good" and "better" in the context of executing a concurrent computation.

Use of a specification language called "Z" has proven useful in making the explicit assumptions used. They began by considering the properties of a stand-alone Occam program running on a network of identical processors, and they tried to identify the restraints which restrict its execution. A specification of a very simple system has suggested a number of points that could be checked experimentally or by simulation. For example: will the subsequent pattern of communications after a process has migrated, settle down to the pattern it would have had if it had started in that configuration from the beginning?

It would be desirable to describe the system analytically and derive quantitative results, but this appears unlikely for such a complex system. Perhaps a very simplified model of the system will represent its behavior sufficiently well to enable conclusions to be drawn in some circumstances. One might conclude that moving a process to another processor would, on the average, reduce delays across the system. The researchers are now looking for measurable properties which might be important in describing system performance, such as synchronization delay between sending and receiving processes, and they are endeavoring to determine the effect that moving one process would have on all the others.

Simulation. A preliminary simulation workbench has been implemented. A set of simulation tools has been produced, on top of which the experimenter produces his own specific model as a simulation program. The idea is to allow the performance of typical computations to be compared on a variety of architectures under a variety of support strategies.

Thus far, a package has been developed which allows different topologies of processors to be built, with parameters controlling the communication delays along links. At the next level, there are components which model the actual strategies employed to represent such system features as process scheduling or message routing.

A number of standard strategies have been incorporated in the model, such as the actual strategy used for generalized interprocess communication on the Meiko Computing Surface (*ESNIB* 88-02:20-33[1988]). Onto this can be placed a network of processes with a communication pattern specified by the user.

These simulations describe the statistical behavior of computations such as the amount of time a process spends in computation before communicating with another, which is determined by a value derived from some probability distribution selected by the user. This program is working, but user programs are only allowed to consist of purely parallel processes at present. It is obviously desirable to include programs in which there is a sequential element as well. There are a number of techniques that might be considered, and this is one of the major additions to be made to the system. However, at this stage, a number of simple experiments can be constructed to examine delays and time spent blocked by the processes, and the end-to-end delay of a fixed computation.

Construction of a Testbed. The main problem in comparing strategies through empirical studies is the difficulty of monitoring activity on such systems in a nonintrusive way. It appears that, in the general case, no system which monitors a distributed computation can guarantee to preserve the communication behavior of an unmonitored program. In particular, any computation involving nondeterminism may be changed quite radically. However, this does not say that the externally observed results will be different. It is essential that nondeterministic programs should preserve externally significant behavior regardless of the internal paths taken. However, since it is necessary to consider internal events as significant in order to improve support, monitoring cannot simply be built into existing systems unless it is permanently switched on during runs.

Adding sufficient monitoring to a system like the Computing Surface, causes unavoidable distortion of internal behavior because of the difficulty in getting noninterfering messages out of the system. Monitoring hardware should be an integral part of any parallel system, and should be incorporated from the beginning. Therefore, Pooley and Candlin are constructing their own parallel machine, laying emphasis on the requirement for monitoring communications along both hard and soft channels, so that the data rate between processes can be derived from measurements of what is happening on hardware buses or to shared memory locations. This parallel engine, a test bed called "Posie" (or Posit), will allow the user to "get inside the hardware" in a way which is normally impossible with commercial machines. In addition to providing information to the operating system, it will also be useful for more traditional performance evaluation tasks.

The machine is based on the Centre Net hardware switched network, which offers very high bandwidth, and an M68000 processor board which can be plugged in as a node. Since the design of the processor boards is complete they should be available by the end of 1988. The next stage is to design the monitor board and to see how to store and process the large quantities of information that can be generated. The board for monitoring bus traffic will sit on a spare node of the Centre Net Starpoint, and send statistical data directly out of the system. The problem of monitoring interprocess communication among processors on the same processor board remains an open question.

In the first phase, the intent is to provide software implementation to measure program characteristics. This is not so desirable, but it will enable making a start and developing a system that can be used on any type of machine. The initial software will be based around an Occam 2 (*ESN* 40-9:306-308[1986]) compiler which will generate profiling code and an operating system kernel which will track communication. Each process and each processor will be able to collect both trace information and cumulative statistics about its behavior.

Other Work. The intent is to put similar software instrumentation on the Meiko Computing Surface, but the facilities for interprocessor communication are very different from those on Centre Net, where all processors are directly addressable. In order to get a consistent picture, there needs to be a uniform process-to-process communication facility which can maintain statistics of traffic between those processes. As a first step, the existing Occam "harness" has been adapted to allow processes to communicate in a way that is independent of their location. The user has to interface his program to the harness by hand, but in principle, this could be done automatically from the source code and the placement statements.

Future Plans. Some of the tasks remaining to be done are to:

- Extend the Occam model to higher levels of detail and produce an outline specification for an operating system that preserves the Occam properties.

- Complete the modeling system so that it will successfully handle run-time deadlock, possibly by implementing a timewarp mechanism with rollback. One final aim is to mount timewarp on the Posie testbed so that existing user programs can be imported. It may be best to build this mechanism into the simulation system.
- Construct a set of experiments to investigate the dependence of overall execution time on such system properties as average synchronization delay or average channel transfer time. It is not obvious what the relevant parameters are, and simulation should provide useful insight. A preliminary requirement is to find ways of generating a set of computations which samples the space of real computations appropriately.
- Get up a number of boards and mount a preliminary version of an operating system so that the hardware can be checked out. Start work on the design of the monitor board and of the software to handle it.
- Produce an Occam 2 compiler with profiling capabilities for the Motorola 68010. Adapt the MUSS operating system so that it can gather statistics of channel usage.
- Continue the work on implementing virtual channels with monitoring capability, and provide software which would handle the interfacing of the user's program to the run-time system.

The long-term goal is to identify those properties of executing parallel programs that can be used for determining good placements. Once this is known, simulation experiments can be conducted to try out migration strategies to find a method of migration that does not cause unacceptable delay to the computation. These strategies could then be incorporated into an operating system that would relieve the user of the responsibility of distributing his program over the parallel machine.

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11/17/88

MATERIALS SCIENCE/SEMICONDUCTORS

NATO Workshop on Metallization and Metal-Semiconductor Interfaces

by Leonard J. Brillson. Dr. Brillson is Manager of the Interfaces and Processing Group, Xerox Webster Research Center, Webster, NY.

The NATO Advanced Research Workshop on Metallization and Metal-Semiconductor Interfaces took place from 22 through 26 August , 1988 at the Technical University of Munich, in the Munich suburb of Garching, West Germany. It included 39 participants from 13 countries including Japan. NATO workshops such as these are dedicated to well-defined and timely, if not time-critical, areas and are constructed to maximize personal communication between participants. The workshop director, I. Batra (IBM, Almaden), ably assisted by F. Koch (Technical University of Munich), achieved great success in providing a stimulating atmosphere to achieve these results. The active participation during the entire meeting of all the attendees owes much to the enthusiasm and attention to detail of these two gentlemen.

The workshop focused on two major issues: metal-semiconductor interfaces and alkali metals on semiconductors.

The scientific talks were grouped as follows:

- General Schottky barrier mechanisms
- Role of defects at metal-semiconductor interfaces
- Metal covalent semiconductor contacts
- Temperature as a barrier mechanism probe
- Barrier manipulation with impurities
- Band offsets and barriers
- Silicon/silicide interfaces
- Application of tunneling to metal/semiconductor interfaces

- Alkali metals/semiconductor interactions – overview
- Alkali-metals/compound-semiconductor interactions (two sessions)
- Observations and group meetings
- Group leaders' reports and general discussion.

The decision to hold an international workshop on these topics derives from the qualitative advances which researchers in Japan and on both sides of the Atlantic have made in the past 2 or 3 years. There were 32 talks, all of which were invited. The distribution reflected the truly international progress that has been made, including talks from the UK (2), France (6), US (9), West Germany (6), Italy (1), Turkey (1), Spain (2), Japan (2), Greece (1), and Switzerland (2).

Metals on Semiconductors – Overview

Professor W. Mönch (University of Duisburg) provided the opening lecture. He observed that it is now 50 years since W. Schottky explained rectification at metal/semiconductor interfaces in terms of a depletion layer on the semiconductor side of the junction. The Schottky-Mott rule followed, e.g., $\Phi_{Bn} = \Phi_m - X_{sc}$ where Φ_B is the barrier to electrons, Φ_m the metal work function, and X_{sc} the semiconductor electron affinity. By 1940, work on metal-selenium contacts made it clear that the dependence on the metal was much less than expected. This was explained in 1947 by John Bardeen in terms of interface electronic states and dipole layers. Fundamental work since then has centered on the physical nature of such states. At the present time, there are a number of physical pictures to account for this Fermi level "pinning" in a relatively narrow range of energies with respect to the semiconductor band gap. These can be grouped into two major categories:

- Continuum of metal-induced gap states, where a charge transfer occurs between the metal and the tails of metal wave functions into the semiconductor in that energy range where the metal conduction band overlaps the semiconductor band gap
- Defect models, where Fermi level "pinning" at the energies of fabrication-induced defects on the semiconductor side of the interface.

Metals on Semiconductors – Experiment

Experimental studies to distinguish between these pictures have employed either device or surface physics approaches. The former are more relevant to technology but are usually ill-defined on a microscopic level. The surface physics approach has yielded considerable new information on an atomic scale, but numerous questions remain about their relevance to macroscopic device contacts. Recently, a number of low-temperature experiments, led by Professor A. Kahn's group at Princeton University, have uncovered evidence for distinctly different behavior between the submonolayer and multilayer regime of metal coverages on a clean semiconductor surface. Furthermore, it appears that more than one mechanism plays a role in the band bending process. Details of the Fermi level movement as a function of coverage now indicate the presence of surface charge centers at band gap energies which relate to physical properties of the metallic (or nonmetallic in some cases) adsorbates and not to the final stabilization energies, which are nearly identical in the case of ultrahigh-vacuum (UHV)-cleaved GaAs (110) surfaces. The energies of the apparent charge state energies at submonolayer coverages have now been correlated with atomic ionization energies (Kahn, Princeton University), electronegativities, as well as interaction parameters within a tight-binding calculational scheme (W. Mönch, University of Duisburg). The low-temperature work has an additional new aspect, namely, the much more uniform surface coverage of the clean semiconductor by metal atoms, in contrast to the island or cluster formation prevalent from metal deposition on surfaces at room temperature. Reflecting the views of many of his colleagues, Mönch concluded that the growth mode of the metal overlayers must be taken into account, especially for large-area measurement techniques such as photoelectron spectroscopy (PES) or Kelvin work function measurement. Furthermore, he concluded that metals induce surface states and dipoles whose character is defined by wave function tunneling into the interface. Deviations from this continuum state model are attributed to fabrication-induced defects.

R. Ludeke (IBM, Yorktown Heights, New York) amplified the theme of defects at semiconductor surfaces – in particular for his delocalization model of impurity states induced by deposition of transition metals on GaAs (110) surfaces. Here rehybridization of Ga and As valence bonds by an additional metal impurity level pushes states into the semiconductor band gap, with states near mid-gap determined primarily by interaction with Ga dangling bonds. With the wave function overlap, the discrete impurity states become a resonance with the entire range of energies shifted due to screening by the metal. Because of the surface character of this impurity, screening is only partial and the resonance maintains considerable defect character (although it is sensitive to the defect-metal distance). In Ludeke's picture, the variation of barrier height with metal work function is weakest for high work function and strongest for low Φ_m. In principle, defect levels must be calculated for every semiconductor, but a single value related to the charge neutrality level of the induced density of interface states (discussed by F. Flores, University of Madrid) or the metal-induced gap states (J. Tersoff, IBM Yorktown). Thus, the defects or impurities generated by the growth process produce levels which are only weakly dependent

on the metal. R. Ludeke argues that this "missing link between MIGS and defect states" can account for the different slopes $S = d\Phi_B/d\Phi_m$ observed experimentally.

Bonding and energetics on Al on clean, ordered Si surfaces was the subject of the presentation by J.S. Nelson (Sandia Laboratories, Livermore, California). Here one can evaluate the surface energies at well-defined surface coverages characterized by low-energy electron defraction (LEED) and scanning tunneling microscopy (STM). As the Al coverage increases, different site coordinations become more favorably energetic along with coverage-dependent bond lengths. F. Koch (Technical University of Munich) noted that epitaxy of Si on Al on Si was in principle possible and speculated that such a structure might have novel electronic properties.

R. Williams (University of Wales, Cardiff, UK) presented results to show that Schottky barrier formation is not easily describable by "linear" models but requires multiple factors whose values may vary from system to system. He described results for Sb on UHV-cleaved InP, a chemically inert interface for which the n-type barrier varied from half the band gap to Ohmic between thin (monolayer) and thick coverages. For Au on CdTe, he showed that two different barriers were measurable at the same contact, with only an electric field stress accounting for the reversible difference. Similarly, two-valued barriers have been measured for Au on CdS and CdTe. Results for metals on oxide-covered CdTe illustrated the importance of near-interface chemistry in forming defect levels which modify the barrier.

In my own talk, I presented PES and cathodoluminescence spectrosopy (CLS) results to show that a Schottky model modified only by defects induced by interface chemical interactions, (e.g. "chemically-induced defects") can account for the wide range of barrier heights now observed for metals on III-V compounds. CLS provides a direct, optical measurement of the interface states and indeed confirms the predictions of a simple electrostatic analysis of the 0.7-eV range of band bending observed by PES for metals on molecular-beam-epitaxy (MBE)-grown GaAs (100) surfaces. I attributed the large contrast between the Fermi level "pinning" for UHV-cleaved (110) GaAs surface (on which the bulk of work at this conference was focused) and the "unpinned" MBE-grown GaAs (100) results to the much higher density of bulk native defects in the melt-grown versus the MBE-grown material. Additional evidence for the influence of bulk native defects on the interface Fermi level stabilization was given using PES and luminescence measurements for metal on CdTe, whose different barriers (including the dual barriers reported by R. Williams) could be related to the observed deep-level defect energies. Conversely, at low temperature MBE-grown GaAs (100) interfaces at which chemical activity could be suppressed, exact agreement with a Schottky model was shown. Similarly, metal interfaces with UHV-cleaved GaP (110) interfaces (at room temperature) exhibited Schottky-like behavior. Apropos to the recent inauguration of the Schottky Institute of the Technical University of Munich campus, the talk concluded with the statement "Schottky was right!".

W. Mönch observed that a wide range of barrier heights is not a proof that the Schottky-Mott rule holds. However, such data presents a challenge for most Schottky barrier models, for which deviations from a central energy level are assumed to be minor perturbations. A notable exception is the work of Duke and Mailhiot (*Journal of Vacuum Science Technology* [1985]), which predicts only minor affects due to interface dipoles, barring extrinsic (i.e., defects, impurities) effects. W.E. Spicer (Stanford University) suggested that two levels reported for the MBE-GaAs (100) interfaces might be due to antisite defects, thereby consistent with a recent extension of his Unified Defect Model. D. Hamann (AT&T Bell Labs) suggested that the Schottky-like behavior for MBE-GaAs (100) versus melt-grown GaAs (110) surfaces may be due to formation of dimerized As on the (100) surface since such a stabilized surface could suppress chemical activity and defect formation.

C. Sebenne (Pierre et Marie Curie University, Jussieu, Paris) described his results for metals on clean, ordered Si (111) surfaces. Here it is possible to obtain ordered, noninteractive overlayers with well-defined dipole formation varying from reconstruction to reconstruction and adsorbate to adsorbate. Overall, a comparison of dipole results is consistent with the difference in adsorbate atom size – large atoms produce large dipoles and vice versa.

W.E. Spicer (Stanford University) surprised almost everyone at the workshop by departing from "heroic attempts to explain everything by one mechanism" and proposing a model which incorporates both MIGS and defects. Here the Fermi level can move away from the canonical MIGS position if the defect densities are high enough. Low-temperature experiments can be used to separate these two factors since low temperature can change the density and type of such defects. The talk focused mainly on low-temperature results for a wide variety of adsorbates on UHV-cleaved GaAs (110) using PES, both synchrotron and ultraviolet. Here considerable discussion arose regarding the separation of n-type and p-type energies at multilayer coverages. Such separation into two discrete levels is regarded as strong evidence for defects but is strongly dependent on the presence of metallic clustering, which can result in spatially averaged energies shifted to slightly higher (n-type) and lower (p-type) energies.

This issue was extended to the criteria for observation of metallization. Spicer argued that spectral features of the PES valence bands were not indicative of the metallization onset, as reported in related low-tem-

perature studies of A. Kahn (Princeton University) and C. Laubschat (Free University, Berlin). These studies were described later in the workshop and interpreted as evidence for Fermi level "pinning" by MIGS. Here initial state effects on the PES energies due to metal clustering (surface charging of small clusters) was used to account for the PES discrepancy. Further evidence for metallization derived from observations of plasmon losses in the PES data at similar coverages. Kahn's discussion of the variation in apparent donor level at submonolayer coverages included a call for realistic calculations of adsorbate-induced states. Such calculations will require a knowledge of adsorbate site and geometry, especially from STM. Kahn also noted that the "real value of low-temperature results depends on the ability to extrapolate to room temperature," where clustering and the density of defects can increase.

Recent PES studies of Si-metal interfaces, using the temperature dependence of reaction and interdiffusion to discuss broad mechanisms of metallization were described by L. Braicovitch (University of Milan). He found that clustering per se is not critical for interface reactions. Rather the presence of metallic screening of interface bonds reduces barriers to reactions. Braicovitch also finds that Gd and Yb can form silicide precursors which can speed up reactions when other metals are deposited. These in turn may be influenced by steric effects.

In a STM session chaired by Nobelist H. Rohrer (IBM, Zurich), R. Feenstra (IBM, Yorktown) described his recent STM observation of adsorbates and metal overlayers on UHV-cleaved GaAs (110) surfaces. These measurements included not only surface morphology on an atomic scale but also barrier measurements from current-voltage studies on a local scale. Feenstra finds that for Sb on GaAs, the clustered surface has different band bending on (versus off) the cluster, confirming the potential problem raised earlier with regard to large-area PES measurements. In addition, he observes additional states extending away from the GaAs band edge into the gap. These states are particularly evident at the edges of the Sb clusters. Feenstra also touched on the difficulty of measurement of few-atom densities-of-states since such clusters are not metallic, making any communication with semiconductor transport states for current-voltage measurements extremely difficult. For Au on GaAs (110), Feenstra observes that dimensional islands of 10-Å height; at a five-monolayer coverage, these islands cover the entire surface and become oriented, twinned crystals. These measurements were a highlight of the conference due to their potential for resolving several of the key issues regarding metallization and electronic states within the band gap.

H. Salemink (IBM, Zurich) described STM morphology and potentiometry measurements on cleaved AlGaAs multilayers by scanning across a cleaved (110) face of the (110)-oriented multilayer film. Salemink combined his STM probe with a scanning electron microscope (SEM) under UHV conditions to monitor the changes in carrier concentration and potential associated with the confinement layers at a p-i-n AlGaAs heterojunction. From a comparison of current-voltage intercepts, he was able to extract heterojunction band offsets in good agreement with published results. This new application of STM adds even more weight to the importance of this technique for understanding semiconductor surface properties.

The use of STM for inverse photoemission spectroscopy (IPS) measurements was described by Bruno Reihl (IBM, Zurich). Incredibly, it appears possible to generate sufficient photon intensity for IPS from atomic-scale surface areas, given the restricted STM current densities and absolute currents. Good correspondence between standard and STM-derived IPS features was shown for Si (111) (7x7) ordered surface. Reihl speculated that rough surfaces may give rise to enhanced photon emission due to plasmon losses, analogous to surface-enhanced Raman scattering, and plans to combine STM-Raman studies on surface-enhanced structures.

Metals on Semiconductors – Theory

M. Lannoo (University of Lille, France) initiated the theoretical presentations regarding Schottky barrier formation by discussing the relationships between barrier heights, heterojunction band offsets and the energy levels of transition metal impurities. Lannoo argued that resonant dangling bonds are equivalent to MIGS and that such dangling bond states explain the relation between barriers, band offsets, and transitive metal impurity levels. Here the success of defect calculations is explained by dangling bonds, which are present even in the presence of defects.

A stimulating talk titled "The Making and Breaking of Barriers with Delta-Doping Layers" was given by F. Koch (Technical University of Munich). With MBE techniques, the researcher has great control over semiconductor doping even at one atomic layer. Placing an abrupt (100 Å) doping layer near a changing potential (i.e., a metal semiconductor interface) results in a "mesoscopic dipole" which can change the barrier height controllably. Thus, for example, $5x10^{13}cm^{-2}$ Sb in MBE-grown Si exhibits no apparent damage with transmission electron microscopy (TEM) and electronic densities are comparable to the doping density, indicating almost full activation. Of course, if the Fermi level is strongly "pinned" at one energy, the "mesoscopic" charge exchange cannot change the barrier, only the charge distribution. Koch presented magneto-transport data bearing the signature of two-dimensional quantum well

structures, as anticipated for these localized dipoles. Future work will now address the barrier problem.

The calculations of electronic orientation-dependent structure and barrier height for Ni- and Co-silicides on Si using a local density functional method were described by Don Hamann (AT&T Bell Labs). He regards these epitaxial silicide-silicon interfaces as ideal systems since they are pseudomorphic, atomically abrupt, with low defect densities as determined from several techniques. He finds significant energy differences in different symmetry structures for both Ni and Co as well as between the two. For Ni, the predicted switch between two of these structures is seen, and its relative ease of occurrence is taken as evidence for small energy differences between symmetry structures. For Co, Hamann predicted poor ballistic transport properties based on the absence of bands near the Fermi level. These transmission predictions have now been confirmed. Hamann regards the Si barrier heights as linear combinations of bulk densities of states of both the silicon and the silicides and can be viewed as MIGS-type states. G.P. Das (Max-Planck Institut, Stuttgart) also described self-consistent electronic structure determinations for the $NiSi_2$-Si interfaces using supercell calculations. Here again, the barrier height difference could be obtained but was derived from the differences between large energy values and only on a relative scale.

F. Flores (University of Madrid) described his self-consistent tight binding approach to interfaces and the concept of Induced Density of Interface States which he developed in 1977. As with MIGS, the interface Fermi level is taken as constant to within 0.1 eV due to resonance states near mid-gap which develop into a broad continuum extending away from the band edges for a fully metallic contact. Flores introduced a new point: that structure in the metal density of states could shift the charge neutrality level in the semiconductor. He also pointed out major differences in barrier height (0.4 eV) for metals on GaAs (110) surfaces, depending on the cation or anion-continued character of the interface bands.

A broad review of his work concerning MIGS, charge neutrality levels, and their application to Schottky barriers and heterojunction band offsets was provided by J. Tersoff (IBM, Yorktown). He argued that while experimentalists were proceeding by induction from specific experiments to general models, theorists in this field were proceeding by deduction from a crucial assumption (Fermi level "pinning" at a charge neutrality level) to explaining deviations from this behavior in specific cases. Tersoff acknowledged that experimental support for his barrier model derived mainly from device measurements, where interface chemistry is poorly understood. Nevertheless, he argued that such measurements represent the most realistic and hence the most important systems of all. Overall, Tersoff concluded that Fermi level "pinning" by MIGS occurs first, followed by other possible extrinsic factors. In considering recent progress, he believes that we are gaining consensus insofar as we are realizing a distinction between high and low coverages, presumably gaining a better perspective of the relationship between surface science and macroscopic device data.

Alkali Metals on Semiconductors – Theory and Experiment

S. Ciraci (Bilkent University, Ankara, Turkey) led off the talks concerned with alkali metals on semiconductor surfaces. These studies provide an important test case for metallization since the alkali metals form abrupt, ordered overlayers, with large surface dipoles with changes in charge transfer and bonding with metal or coverage which can be analyzed in detail. Recent agreement between theoretical calculations of S. Ciraci and I. Batra versus those of M. Tsukada (University of Tokyo) for K on Si (111) (2x1) surfaces adds support for the approaches taken in the past year. M. Tsukada devoted considerable attention to the comparison between "metallic" plasmon appearance and dipole evolution at similar coverages. Several workshop participants expressed caution at the interchangeable use of polarization charge and bonding charge to describe the same charge redistribution phenomena.

The inconsistencies in dipole voltage versus coverage measurements for K on Si (100) (2x1) surfaces were addressed by R. Miranda (University of Madrid). He showed nicely from thermal desorption spectroscopy data that the thermal desorption extends to room temperature. Thus, the saturation coverage around room temperature depends critically on the exact temperature. Small differences in "room temperature" from one laboratory to another could therefore account for the significant apparent discrepancies.

P. Soukiassian (University of Paris, Orsay) described recent work for Na on Si (100) (2x1) surfaces, where it was concluded that the Na-Si bond is weak, covalent, and derived from the Si dangling bond. However, controversy arose concerning the interpretation of PES core level shifts. L. Braicovitch (University of Milan) pointed out that the absence of a large chemical shift in the core levels was not in itself proof of small charge transfer.

I. Batra (IBM, Almaden) made the point that theorists can calculate charge transfer in the alkali metal-semiconductor systems with confidence, but have no easy way to integrate it properly because of the complex charge rearrangement in the surface.

Conference Summaries

The workshop included a wrapup evaluation of the results achieved and future progress. Hamann made the

proposition that "theory and experiment can only meet when the interface atomic geometry is well-defined." Here, the silicide-silicon interface represents such a well-ordered reproducible contact. He also asked whether we can controllably span the range from MIGS-dominated contacts to Schottky-dominated contacts. Spicer called for more precise barrier measurements and model-specific calculations (0.1-0.05 eV) on interfaces for which the chemical composition is known in detail. The need for well-defined interfaces – either through epitaxy, surface passivation, judicious selection, or merely brute force characterization on an atomic scale – was expressed in a variety of forms by many workshop participants. Batra added that we need systems which can span the range from ideal to real systems. Flores expressed the belief that model calculations have enough flexibility to take the details of real metal-semiconductor interfaces into account. There was general agreement that no one mechanism dominates metal-semiconductor contacts. No single model can explain all the available data. There was full agreement that theory has the capability to address the nature of bonding and charge transfer, particularly for alkali metals on semiconductors.

Concluding Remarks

In summary, the NATO Advanced Workshop on Metallization and Metal-Semiconductor Interfaces achieved among its diverse participants a consensus of thought not obtained in any other of the topical conferences I have attended. The proceedings of the workshop will appear in book form in early 1989 as part of the NATO ASI Conference Series. Interested readers should contact, Dr. Inder Batra, IBM Almaden Research Laboratory MS K33-801, San Jose, California 95120.

11/25/88

Structure-Property Relationships in Ion Beam Surface Modified Ceramics: Theory and Applications Presentations at a NATO Advanced-Study Institute

by Fred Smidt. Dr. Smidt is the Head of the Surface Modification Branch at the Naval Research Laboratory in Washington, D.C.

Introduction

This 2-week NATOAdvanced Study Institute was held from 28 August through 9 September 1988, at Il Ciocco, Italy, a conference center in the Tuscany foothills about 60 miles north of Pisa. The conference was organized by Carl J. McHargue (Oak Ridge National Laboratory, Tennessee) with assistance from codirectors Ram Rossowsky (Pennsylvania State University, State College, Pennsylvania) and Wolfgang O. Hofer (Kernforschungsanlage, Jülich, West Germany) on the subject of modification of properties of ceramics by ion beam processing. Initial investigations of ceramics have shown many differences in their response to ion bombardment from those observed to occur in metals, and the intent of the conference was to examine the reasons for these differences. The conference attracted many investigators from those groups active in ion implantation of metals, and many of the participants also attended the International Conference on Surface Modification of Metals by Ion Beams held the following week in Riva del Garda, Italy. The conference format, as with all NATO institutes, had lecture sessions morning and late afternoon with extensive time for interaction and discussion among the participants. Invited lectures of 2-hour duration were presented by 17 speakers; shorter current research highlights were presented by 21 others out of the 70 participants. The conference was a very pleasant way in which to get an update on the emerging field of ion beam modification of ceramics.

Ion Beam Effects in Ceramics

C.R.A. Catlow (University of Keele, UK) opened the institute with a review of defects and defect aggregates, which are observed to be stable in ceramics, with particular emphasis on those stabilized by the requirements to maintain charge neutrality, which are not encountered in metals. The various approaches to simulating and computing defect properties were then covered with applications to correlated defect motion in Li_3N, stable defects in alkali halides, and defects in perovskite superconductors.

The basic theories for damage production in multicomponent ceramics were reviewed by Don M. Parkin (Los Alamos National Laboratory, Los Alamos, New Mexico), who noted that no model exists for the complete treatment of a real material. Computer simulations of the effects of displacement threshold, elemental mass ratios, stoichiometry, bonding type, and bombarding particle and energy on the damage produced have been studied. The problem becomes particularly complicated with large mass ratios (e.g., Ta_2O_5), with different threshold displacement energies for anions and cations, and where material stoichiometry does not match the cascade stoichiometry. Guidelines were provided to estimate regimes in which "normal" cascade behavior would be observed.

Jorgen Schou (Riso National Laboratory, Roskilde, Denmark) continued the discussion of complexity of the cascade processes in ceramics with a review of sputtering in ceramics. In addition to complexities discussed by Parkin from ballistic collisions there is also a sputtering component due to electronic excitations produced in insulators by the energetic ion. Electronic sputtering correlates with the electronic stopping power, but there appear to be multiple mechanisms by which de-excitation can occur and they are materials dependent.

A very good review of the ion beam mixing field including basic ballistic recoil mixing, marker experiments, temperature dependence of mixing, and chemical effects in the thermal spike was given by Franz W. Saris (Institute of Atomic and Molecular Physics [F.O.M.], Amsterdam, the Netherlands). Strong evidence for the existence of chemical effects during the 10^{-12}-second thermal spike of the cascade was presented, with the extent of mixing in various alloy systems shown to be a linear function of $\Delta H_{mix}/\Delta H_{cohesion}$. The critical temperature at which radiation-enhanced diffusion contributes to mixing was also shown to correlate with the cohesive energy of the alloy because of the relationship to the defect creation energy. Finally, Saris discussed the prediction of metastable phase formation in the cascade and recent comparisons with other rapid quenching techniques in the Ni-Ti system. More than just rapid cooling in the spike appears to be involved since different phases and different composition regimes for stability were observed for ion mixing and splat cooling. Only a few ion mixing experiments have been performed on ceramic systems except for silicide contact studies.

Paul Thevenard (Claude Bernard University, Lyon, France) presented a review of defects produced in alkali halides simple oxides by ion bombardment, pointing out in particular that a number of electronic processes contribute to defect formation in these materials. Experimental studies of the defects produced in LiF, MgO, TiO_2, and Al_2O_3 using optical absorption, TEM, X-ray, and Mossbauer spectroscopy to characterize the defects were reviewed. Studies of adhesion of metal films to Al_2O_3 and amorphization of the various materials were also described. The experimental results were all taken from work done at Lyon.

Applications of Ion Beam Processing

Carl McHargue (Oak Ridge National Laboratory, Oak Ridge, Tennessee) reviewed the phenomena associated with ion beam mixing of a metal film into a ceramic substrate with particular attention to applications for improved adhesion. The situation is much more complex for ceramics than for metals because of the difference in displacement energies for the oxygen and metal sublattices, and the formation of stable complexes and compounds which do not diffuse easily. The mechanical properties of implanted ceramics have been studied extensively and indicate an increase in toughness in the surface layers for Al_2O_3 as indicated by crack curvature near the surface for cracks produced by a microhardness indent. Bend tests of polished Al_2O_3 also showed a decrease in the frequency of failure for a given load. Microhardness tests on ceramics made at low loads with the nano-indenter were found to be misleading because of elastic recovery of the indent depression so that the measured area was much less than the actual area at the point of maximum load.

The chemical properties of ceramics and the tailoring of chemical properties by implantation, ion beam mixing, and ion-beam-assisted deposition (IBAD) was reviewed by Gerhard K. Wolf (University of Heidleberg, West Germany). A number of examples of corrosion protection using films deposited by IBAD showed very good results, particularly one for CrN that survived 50 d in a seawater immersion test. Implantation of ceramics appears promising for enhancing catalytic activity, but oxidation protection is a strong function of the chemistry and structure of the material. Amorphous SiC oxidizes at twice the rate of untreated SiC.

Peter D. Townsend (University of Sussex, Brighton, UK) reviewed the use of ion beam processing to modify the optical and electrical properties of insulators and their use to fabricate wave guides and electro-optic devices. A major effect is the damage produced by nuclear collisions which can amorphize materials such as silica glass and lower the refractive index. Implantation to change the composition can also be used to modify the optical properties but suffers from losses due to absorption centers and shifts in composition due to preferential sputtering. An important new finding is that the poling temperature for $LiNbO_3$ can be reduced from 1140°C to 600°C by excitation of the crystal with a 1-MeV electron beam during the application of the poling voltage. The fabrication of wave guides in crystalline quartz by ion bombardment and the fabrication of electro-optical and

acousto-optical devices was also discussed. Chris Buchal (KFA, Jülich, West Germany) and T. Bremer (Osnabruck, West Germany) presented additional work on implanting Ti into $LiNbO_3$ to produce wave guides, modulators, and switches for integrated optics.

My own paper was a review of the technique of ion-beam-assisted deposition (IBAD) in which a thin film is deposited by vapor deposition during simultaneous ion bombardment. Improvements in film properties such as higher density at low deposition temperatures, improved adhesion, modification of the grain structure, and reduction in epitaxial temperature were discussed and shown how they can lead to improved performance in applications such as wear, corrosion protection, optical thin films, and adhesion.

A. Antilla (University of Helsinki, Finland) reviewed the production of hard carbon films by ion beam and plasma processes and their use for wear resistance, corrosion resistance, and improved thermal conductivity. J.T.A. Pollock (CSIRO, Research Laboratory, Lucas Heights, Australia) presented related information on the implantation of polymeric carbons to increase wear resistance and T. Hioki (Toyota Central Research Laboratory, Aichi, Japan) described a process for applying hard carbon films to SiC, Si_3N_4, and Al_2O_3 ceramics to produce low friction and improved wear resistance films.

The final speaker of the program was Mike Nastasi (Los Alamos National Laboratory, Los Alamos, New Mexico) who described the use of ion beams for characterizing the new high T_c ceramic superconductors and for patterning them to produce devices by amorphizing the ceramic.

Conclusion

The surface modification of ceramics by ion implantation and the deposition of thin films on ceramics by ion mixing and ion-beam- assisted deposition promises to be the primary growth area in ion beam processing of materials over the next 5 to 10 years. This conference provided a good introduction to the fundamentals of the field and a glimpse at promising applications and current research. The proceedings will be published as a NATO-Advanced Study Institute monograph by Martinus Nijhoff Publishers near the end of 1989 and should provide a good reference for researchers in the field or those contemplating entering the field. Individual reprints should be available from the individuals cited.

11/30/88

MATHEMATICS

The European Consortium for Mathematics in Industry (ECMI) and the ECMI 88 Conference

by Richard Franke. Dr. Franke is the Liaison Scientist for Mathematics and Scientific Computing in Europe and the Middle East for the Office of Naval Research European Office. He is on leave until September 1989 from the Naval Postgraduate School, Monterey, California, where he is a Professor of Mathematics.

The ECMI

There is a general need for increased cooperation between mathematicians in academic positions and industry. After the "David Report" (1984), which noted that "Too few people recognize that the high technology so celebrated today is essentially a mathematical technology," a group of European mathematicians began to discuss the problem and possible solutions. As a result, the first European Symposium for Mathematics in Industry was organized (with financial help from the European offices of ONR and EOARD and others) and held in Amsterdam in late 1985 (Hazelwinkel et al., 1988). As a result of discussions which took place then, an organizational meeting was held at Neustadt-Massbach, West Germany, in April 1986, and in March 1987, at Oberwolfach, the second symposium. In June 1987, the European Consortium for Mathematics in Industry (ECMI) was formed as a legal entity. The first president was Dr. Michiel Hazewinkel of the Center for Mathematics and Computer Science, Amsterdam.

The major objectives of ECMI are: (1) to promote the use of mathematical models in industry; (2) to educate "industrial mathematicians" to meet the growing demand for such experts; and (3) to operate on a European scale

(Wacker). To achieve these goals, ECMI plans to provide, through its academic members, several services to industry. Included among these are:

- Problem identification and formulation
- Identification of expert advice
- Problem development and solution
- Training of graduate mathematicians
- Further training of industrial staff
- Encouragement of students to seek careers in European industry.

Industrial members of the organization have access to a number of services, including free initial advice on problems, after which the company may be put in touch with an appropriate expert, and the opportunity to present problems for solution during the course of the academic postgraduate program.

There is great emphasis on multicountry projects, and indeed there is a great deal to be gained from these, since areas of mathematical expertise of the European countries are often complementary. Examples of this cooperation are seen in several large projects which are currently underway, and which, to a certain extent, may be precursors of what will happen in many areas as the economic barriers between the EEC countries are removed in 1992. In addition to research cooperation, the consortium also has established a 2-year postgraduate program with the goal of providing mathematicians and other university graduates in related fields with the educational training necessary for a successful industrial career. By cooperation between universities in different countries they intend to provide a network of academic groups which will cover all areas of applications of mathematics to industrial problems. A part of the program is the necessity that the student spend at least one semester in another country. For graduation, a thesis on an industrial topic is required and the student will spend up to 6 months working in industry. So far the program is operational at the Universities of Oxford and Strathclyde in the UK, Eindhoven (the Netherlands), Kaiserslautern (West Germany), Linz (Austria), and Bari and Florence (Italy).

ECMI 88

The third scientific meeting of the consortium, the European Conference on Mathematics in Industry 88 (ECMI 88), was held at Strathclyde University, Glasgow, 28 through 31 August 1988. The meeting was attended by about 200 academic and industrial mathematicians (about 10 percent from industry). The tone of the meeting and presentations was generally very applied-oriented, often with speakers citing particular industrial problems as the motivation for their studies. There were nine invited presentations of 40 minutes each, three 90-minute minisymposia, and about 75 contributed papers of 20 minutes, with 5 minutes allotted for questions between talks. Each minisymposium was organized around a particular problem, or around a particular research group. Even though the contributed papers were organized in three parallel sessions, this meeting ran on a long, tight schedule. I will review several of the talks to indicate the flavor of the meeting.

The Overview Paper

The lead talk was presented by the current president of ECMI, Professor Helmut Neunzert of Kaiserslautern University. His paper, "Industrial Mathematics – Aspects of a European Cooperation," gave a survey of the activities of the consortium, and concluded with a case example of the kind of cooperation between countries and industry that ECMI is attempting to foster. Professor Neunzert reiterated some of the observations in his "Letter from the President" (Neunzert, 1988). While ECMI is apparently well on the way to achieving many of its goals, Professor Neunzert noted that there are a number of persistent difficulties, mainly with the industrial "partners." The industrial companies are fearful that such cooperation will result in the transfer of company confidential knowledge to competitors; they are ignorant of the benefits that broader mathematical expertise than available in-house can bring to bear on their problems; and they suffer simple bureaucratic inertia. Companies tend to use the kind of mathematics that has proven useful before and often do not seek new solutions nor applications to new areas. A broad base of mathematical expertise can result in advice such as "I don't know the solution to your problem, but I know someone who can solve it." On the academic side, it might be noted that historically, many mathematicians have been reluctant to dirty their hands with real-world problems, although such persons are probably not participating in ECMI. The arguments for cooperation among various academic groups in the European community and industrial organizations are easy to make, since new technology does require solving complicated problems, and even old technology needs to be used in an optimum way.

As an example of the kind of cooperation that can be brought to bear on a problem, Neunzert outlined a particular example of work in progress. The problem under study was high altitude (about 100 km) flow about the European space shuttle, the HERMES. The problem involved both the Boltzmann equation as well as the Navier-Stokes equation, and was considered as four interrelated parts:

1. A three-dimensional simulation model was to be developed. This model would necessarily be run on a vector computer, so needed to be highly vectorizable. Professor Neunzert's group at Kaiserslautern worked on this part of the problem.

2. It was necessary to develop and apply suitable boundary conditions. Professor Cercignani of Milan University was in charge of this part.

3. A domain decomposition scheme was used to treat the Boltzmann and Navier-Stokes regimes, and Professor Bardos at Ecole Normal Superieure and his group were in charge of this effort.

4. The simulation involved a "game" which was to be the "same" as the natural phenomenon, but not a simulation of nature. This involved collision models, which were developed by Professor Kuscer of Ljubljana, Yugoslavia.

It might be noted that the cooperation with Eastern Block countries (which the organization, or at least some of its members, seek) is not popular with either the industrial partners nor West European governments.

Simulated Annealing. Another interesting invited paper was that given by Dr. Peter P.J.M. Van Laarhoven of Phillips Research Laboratories, Eindhoven, whose paper was titled "Simulated Annealing: Theory of the Past, Practice of the Future?" Simulated annealing is a way of obtaining reasonable approximate solutions to large combinatorial optimization problems. The name arises from a simulation of the process of annealing, wherein slow cooling of (say) a metallic object reverts to its lowest energy state. The primary application discussed in this talk was that of locating the elements (a certain number of modules, with certain given connections) on an integrated circuit chip. The objective function to be minimized is the area of the circuit, small circuits being faster and (perhaps more important commercially) the yield (or percent of the circuits that are good) is inversely related to the area of the circuit. The problem is non-polynomial (NP) hard, which means as a practical matter that the solution is prohibitively expensive to obtain for circuits with a large number of modules and connections. However, the optimum solution is probably not much better than many other configurations which are much less expensive to obtain. So, the process of simulated annealing is applied to the problem. An initial configuration is specified, and then "nearby" configurations are considered. The process of simulated annealing will accept any proposed configuration which decreases the objective function, but will also accept some configurations even though the objective function is increased.

The mechanism for the transition from the current "best" configuration at stage i to that at a later stage, j, is as follows. Let c_i and c_j be the values of the objective function for the configurations at stages i and j, respectively. The configuration at stage j is accepted as the new "best" configuration if $c_j < c_i$ (with probability one), but may also be accepted if $c_j \geq c_i$ (with probability $\exp((c_i-c_j)/c)$). Here c is a parameter which can be interpreted as the rate at which cooling occurs and which decreases as the number of iterations (the number of configurations considered) increases. The details of obtaining nearby configurations was not completely spelled out, but in the linear (or one-dimensional case) simply involved pairwise swapping of the modules. In two dimensions, translation, rotation, and swapping of modules is considered, along with other possibilities. According to the speaker, the process is asymptotically effective, meaning that the process can find the global minimum of the objective function with probability 1. As a practical matter, however, this depends on the process of obtaining the configuration for the next iteration, and the behavior of the parameter c, and suitable choices of these are made empirically. Van Laarhoven has recently written a book on the subject (Van Laarhoven, 1987).

Supercomputers. Dr. Iain S. Duff of the Harwell Laboratory, UK Atomic Energy Authority, gave an invited talk, "Supercomputers." For purposes of the discussion, he considered supercomputers to be general purpose machines with a small number of processors capable of a peak execution rate in excess of 500 Mflops. Thus, machines with many processors and novel architectures were not considered even though such machines may be capable of such peak instruction rates. The definition of a supercomputer is necessarily dynamic; other people have defined a supercomputer as the most powerful machine available at any given time.

After a survey of the numbers and types of machines at various facilities in Europe (there are a total of about 80 in Europe), the discussion turned to the need for and use of this kind of computing power. The primary example given was the use of the Harwell fluid dynamics code, FLOW3D, to simulate (albeit, crudely) the disastrous King's Cross subway station fire, which occurred on 18 November 1987. The entire escalator tunnel and booking hall for the Victoria line, including entrances and exits, but excluding the ticket booths, was modeled. The fire was simulated by a heat source; the combustion process was not simulated. The real time simulated was only a few minutes (firemen arrived while the fire was very small, about 2 minutes before it erupted into a major conflagration), but the computation took 48 hours of cpu time on a Cray 2 computer. The results of the simulation are part of the official record of the inquiry, and have not yet been released, although a synopsis of the results have been made public ("King's Cross Enquiry," 1988) The calculations gave significant insight into the reasons the death toll was so high. What was revealed by the computation was that the distribution of temperatures near the heat source was not as would be expected after casual consideration. Instead of the heat rising to the top of the escalator tunnel and causing the highest temperatures to be there, the heat flow, in fact, was near the bottom, along the escalator steps. The tube, acting essentially like a blowtorch, resulted in a high-velocity air flow through the escalator tube and into the booking hall (this is referred to as a trench, or chimney, effect). A videotape giving a

three-dimensional view of the facility, with color-coded temperatures, illustrated the progression of the heat up the escalator tube. The results of the Harwell calculations were subsequently used in designing a one-third-scale experiment, which confirmed the basic results of the calculations. Without a supercomputer, this calculation could not have been performed (and indeed, this was perhaps, even then, near the limits of being reasonable to do). So, the primary message is that access to a supercomputing facility allows one to investigate situations which in the past one could only speculate about. This is not a new message since that has been said since the advent of the electronic computer.

Problems Concerning Electrical Transmission Lines. Finally, I mention one of the more successful mini-symposia, illustrating cooperation across country borders, which was organized by Professor Robert Mattheij of the Technical University of Eindhoven. The group of three talks all treated different aspects of the same problem, which was illustrated by the initial showing of a videotape. The problem concerns electrical transmission lines, and mostly the wind-forced vibration of them under various assumptions about the forming function and the way the lines are suspended. Problems such as the dynamic load readjustment due to a hanger breaking and electrical transients caused by lightning strikes also been considered, but were not discussed here.

The first speaker was Professor Peter Hagedorn of the Technicsche Hochschule Darmstadt. He said that in West Germany, the costs of maintaining transmission lines are as expensive as generation of the power, so it is worthwhile to consider ways of decreasing these costs. He described the part of his research in modeling the steady response of the lines, looking at two different ranges of vibrations – so-called "galloping" vibrations at a frequency of 0.1 to 1.0 Hz, and vortex excited oscillations at 10 to 100 Hz. The steady-state differential equations for the suspended wire are solved. For the vortex-excited frequencies, the set of natural frequencies is very dense, with a spacing of about 0.1 Hz. Definitive results await the estimation of a number of parameters, which will be done by experimental tests being performed at Buren, West Germany.

The second speaker was Professor S.W. Rienstra of Technical University of Eindhoven. Since he is primarily interested in the "galloping" mode, he considered the vibrations of coupled spans of suspended cables. Because the source parameters of his model were weak and the aerodynamic properties of the cables unknown, the free vibrations were first considered. The model was constrained to planar motion, although the hangers were allowed to move freely. In experiments, it was only possible to measure the tension in the hangers, and from these it was desired to deduce the displacements. Since the equations include many modes it was very difficult to obtain nearly periodic solutions. An asymptotic analysis was performed, which turned out to be quite interesting in that it predicted tension-displacement relations which had been measured experimentally, but until then regarded as being erroneous.

The final speaker of the session was Professor A.H.P. Van de Burgh of the University of Technology, Delft. He considered galloping oscillations of simple elastic structures. The model was a cylinder suspended on springs driven by steady, uniform horizontal fluid flow perpendicular to it. This system was simplified by assumptions about the drag and lift forces on the structure in terms of the relative flow velocity and angle of attack of the flow relative to the structure. The resulting equations are autonomous and weakly nonlinear. These equations were studied analytically using standard perturbation and projection methods. One result, physically observed in the "galloping" phenomenon, is that under certain conditions all horizontal oscillation is damped out.

Conclusions

This meeting provided an impressive display of inter-country and industrial-academic cooperation. If this is indeed a precursor of things to come, then the European scientific community members will become even more powerful as they continue to join forces. The proceedings of the meeting will be available (McKee, 1989).

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11/18/88

PHYSICS

The 1988 International Conference on Defects in Insulating Crystals

by W. Beall Fowler. Dr. Fowler is in the Department of Physics and Sherman Fairchild Laboratory at Lehigh University, Bethlehem, Pennsylvania.

The 1988 International Conference on Defects in Insulating Crystals, held at Parma, Italy, from 29 August through 2 September 1988 was the eleventh in a series which began in 1956. There were 260 participants, from 32 countries at this meeting which was chaired by Rosanna Capelletti of the University of Parma. The Proceedings, consisting of the 22 invited lectures, will appear in the journal *Crystal Lattice Defects and Amorphous Materials*.

These conferences have greatly expanded in scope since their original concentration on color centers in alkali halides. This time less than one-third of the abstracts involved alkali halides, while the remainder treated a wide variety of insulating solids. Oxides of many types were heavily represented (however, only a few papers on the superconducting oxides appeared).

This conference followed the pattern of recent ones in bringing together two areas: optical properties (typified by color centers) and ionic transport (typified by fast ion processes in oxides). The necessity of parallel sessions prevented me from attending many of the sessions on transport. I did, however, attend plenary lectures on this topic.

The study of defects in insulating crystals rests on a firm base of concepts, facts, and techniques developed through the early 1970's. As scientists strive to develop defect models for complicated systems (as, for example, oxide defects near the interface in silicon-dioxide/silicon capacitors), it is important to remember that many of the ideas being considered (large lattice relaxations, charge-dependent atomic configurations, for example) were developed and tested on simpler crystalline systems such as alkali halides. Even now, the physics of deep levels in semiconductors owes much to the concepts developed in the color center field. Nature has been kind in providing us with insulating crystals which are simple enough that high-quality basic physics can be carried out on them, and we should continue to exploit that fact as thoroughly as possible.

Transport

Much of the recent progress in ionic transport has involved development of theory in close collaboration with experiment. For example, P.A. Cox and C. R. A. Catlow of the University of Keele (UK) are using extended x-ray absorption fine-structure spectroscopy (EXAFS) in connection with molecular dynamics to analyze the structural and dynamical properties of mixed cation fluoride conductors such as $Rb_{1-x}Bi_xF_{1+2x}$. Others are also using molecular dynamics; for example, D. A. MacDonaill of Trinity College, Dublin (Ireland) and P. W. M. Jacobs and Z. A. Rycerz of the University of Western Ontario, London (Canada) are studying the fast-ion conductor delta-bismuth oxide.

Other theoretical developments related to transport include the improvement of quantum-mechanical embedding techniques, as typified by the work of J. H. Harding and others at Harwell Laboratory (UK). Further relevant theoretical techniques were discussed by J. M. Vail of the University of Manitoba (Canada), in collaboration with A. B. Kunz at Michigan Technological University, Houghton, Michigan. An important recent development is the consideration of entropy effects associated with defect formation and migration, discussed by Jacobs.

Dielectric relaxation has for some time been an important tool in analyzing defect properties in complex insulators. Here again, the combination of experiment and computer simulation is providing insight into the physics. A paper by S. Ling and A. S. Nowick of Columbia University (New York), A. N. Cormack of Alfred University (Alfred, New York) and Catlow showed how such techniques have established the nature of the intrinsic defect in MnF_2 to be an anion Frenkel defect.

Although high-temperature superconductivity does not involve ionic motion, it does involve oxides, and several papers were presented on perovskite-related oxides which suggested relationships which might be relevant in

understanding these materials. D. M. Smyth of Lehigh University, Bethlehem, Pennsylvania, presented an invited paper on interrelationships of the structures of various perovskites.

An important new technique for studying defects and disorder in ionic materials, quasi-elastic diffuse neutron scattering, was discussed by M. T. Hutchings of Harwell.

Spectroscopic Studies

The properties of excited defects continue to be of great interest and excitement. F. Luty, F. Rong, and coworkers at the University of Utah, Salt Lake City, have over the past few years discovered several remarkable properties involving energy transfer from electronically excited defects to internal vibrational modes of nearby molecules. Perhaps the most spectacular of these is the transfer of some 1 eV of energy from an excited F center (an electron trapped at an anion vacancy) in CsCl to the $n = 4$ or 5 stretching vibration of a neighboring CN^- ion, which then emits vibrational luminescence, slowly cascading to the vibrational ground state. Luty has shown that this system can be pumped and that laser action is possible. The physics of the energy transfer process from F center to CN^- is not at all well understood. At the conference Luty reported similar highly efficient energy transfer from excited F centers to vibrationally excited OH^- ions several lattice constants away. The OH^- ions, however, decay nonradiatively to their vibrational ground state.

These are but a few of the important processes which can be studied in connection with molecular defects. As the concentration of molecules increases, interaction effects become increasingly important. This has been demonstrated by Luty and others using substitutional CN^- ions in alkali halides. In fact, as shown by P. Wochner, E. Burkel, and J. Peisl of Ludwig-Maximilians University, Munich (West Germany), such a system behaves as an orientational "spin glass," and studies involving the coherent quasi-elastic diffuse scattering of thermal neutrons allow one to analyse the nature of the glass transition.

Other excited-state processes include the creation of F centers by ionizing radiation in alkali halides. Here, subpicosecond optical spectroscopy on the excited state of the crystal (the self-trapped exciton) has shown just how the creation process proceeds. R. T. Williams of Wake Forest University, Winston-Salem, North Carolina and N. Itoh of Nagoya University (Japan) have pioneered this research, which is also being carried out by other groups, and recent theoretical calculations by K. S. Song at the University of Ottawa (Canada) suggest just why the self-trapped exciton becomes unstable to the formation of an F center and a neighboring H center (a halogen$_2$ molecule at a single halogen site).

Similar instabilities in other excited-state systems are likely to occur, but they have not been studied in such great detail. One important case is silicon dioxide, where Itoh and others have shown that absorption of ionizing radiation leads to an enormous relaxation of oxygen atoms, forming a transient oxygen vacancy nearby a triplet oxygen molecule. In most cases the system subsequently returns to the ground-state atomic arrangement, often after luminescence occurs, but occasionally (particularly in amorphous silica) the defect becomes permanent.

Another intriguing spectroscopic property, discussed at the conference by D. Schmid of the University of Düsseldorf (West Germany), is superfluorescence, the spontaneous collective emission of coherent light from an ensemble of excited two-level systems. This has been observed to exist in connection with O_2^- centers in KCl. This phenomenon had not been previously observed in solids, and Schmid's measurements call into question certain assumptions made in the initial theory of the phenomenon.

Other new spectroscopies presented at the conference include the use of three-photon absorption to study the exciton and band-gap regions in alkali halides. This work, by D. Frohlich and coworkers at the University of Dortmund (West Germany), provides important new information since the selection rules for the simultaneous absorption of three photons differ from those for one- and two-photon processes. Frohlich's studies in several alkali halides reveal the polariton structure, which yields the energies of transverse and longitudinal excitons, as well as other band-structure parameters.

Applications

Probably the most important applications of the study of defects in insulating crystals involve the concepts and ideas which continue to emerge from this field, influencing the study of semiconductors, complex insulators, and glasses. This is a logical and central feature of fundamental scientific studies of simple systems.

There have been, and continue to develop, direct applications of this research. Widely cited in the past were solid-state radiation detectors, phosphors, silver halide photographic materials, and solid-state batteries involving fast ion conductors. More recently, the color-center laser has gained in practical importance as its spectral range and performance have improved. A number of papers at the conference addressed laser properties and development; for example, G. Baldacchini of the ENEA Laboratory at Frascati (Italy) reviewed recent developments concerning one class of color center lasers, those based on F_A centers (an F center adjacent to a cation impurity).

In addition, an entire session of invited papers was devoted to applications. In the first of these H. von Seggern of Siemens AG, Erlangen (West Germany) discussed the physics and medical applications of x-ray storage phosphors. At present, RbBr:Tl and BaFBr:Eu are the materials of commercial interest, and the storage and recovery processes of these phosphors are directly related to the color centers in these materials.

P. D. Townsend of the University of Sussex, Brighton (UK) discussed ion implantation in electro-optic materials. This process can be used to change the electro-optic properties in a controlled manner; it can also have the deleterious effects of introducing color centers and of decreasing chemical stability. It can also cause amorphization which, however, can be advantageous in certain circumstances.

While most papers at the conference emphasized bulk defects, W. Gopel of the University of Tübingen (West Germany) discussed surface defects and their exploitation for gas sensing. This topic brought a distinct "chemical" flavor to the conference as, for example, the absence of an atomic oxygen at a TiO_2 surface can affect the reactivity of that site with oxygen molecules.

That the photographic process is still the subject of fundamental scientific study was attested to by a paper by R. S. Eachus and M. T. Olm of Eastman Kodak, Rochester (New York) on the role of ionic defects in the radiation physics of silver halides and their exploitation in photography. While most aspects of the photographic process are reasonably well understood, the detailed atomic structure of shallow effective-mass traps is still not certain, and certain defects seen in single-crystal silver halides are not apparent in emulsion microcrystals. Some of these issues were addressed by others at the conference, including a talk by L. Slifkin of the University of North Carolina, Chapel Hill, on the physics of lattice defects in silver halides.

The final "applied" talk addressed a rather different issue, namely, that of radiation damage of fusion materials associated with high-temperature electron irradiation. Here E. R. Hodgson of the EURATOM/CIEMAT Fusion Association, Madrid (Spain) outlined the difficulties of choosing suitable electrical insulating materials for fusion reactors, materials which can remain stable during prolonged irradiation. Relatively little data has been obtained to date on materials exposed to irradiation similar to that which will be present in future fusion reactors, and what data exist suggest a number of likely problems, including radiation-enhanced electrical breakdown, which may be related to radiation-enhanced impurity diffusion. The possible deterioration of other properties such as thermal conductivity and mechanical strength have not been considered in any detail as yet.

Summary

The Parma conference, through an extraordinarily well-chosen program and an excellent mix of conferees, demonstrated again the versatility and richness of the field of defects in insulating crystals. It also demonstrated that with a few outstanding exceptions (primarily the work of Fritz Luty) the scientific strength of this field lies outside the US. The effects of the decision made in the early 1970's by US funding agencies to no longer support fundamental studies of defects in alkali halides are now quite apparent.

It should be noted as well that the nonscientific aspects of the conference were outstanding, as befits a conference held in Parma, the jewel of the Emilia-Romagna section of Italy.

11/26/88

The 10th International Cloud Physics Conference

by Richard K. Jeck and James W. Fitzgerald. Drs. Jeck and Fitzgerald are from the Atmospheric Physics Branch of the Naval Research Laboratory in Washington, DC.

This conference, held from 15 through 19 August 1988 in suburban Frankfurt, West Germany, was one of a series which meets quadrennially. It is the big meeting for cloud physics, however, and this year it drew 300 or so attendees from around the world.

Eighteen oral sessions and two poster sessions filled up the 5-day meeting. The sessions were organized along the following topics:

- Cloud Microphysics: laboratory studies, field measurements and theory, entrainment and mixing, numerical modeling

- Clouds and Radiation
- Cloud Chemistry and Acidic Precipitation: measurements and numerical modeling
- Instrumentation
- Orographic Clouds
- Cirrus Clouds
- Boundary Layer Processes, Fogs and Layer Clouds
- Cyclones, Fronts, and Rainbands
- Graupel and Hail
- Convective Clouds: measurements and theory, and numerical modeling
- Severe Storms and Thunderstorms
- Satellite Studies

A two-volume, 724-page set of preprints has been published by Deutscher Wetterdienst, Frankfurter Strasse 135, D-6050 Offenbach am Main, West Germany.

Trends

During the past 20 years there has been a strong increase in numerical modeling studies, but a sharp decrease in laboratory investigations of basic microphysical processes. The number of field projects has increased modestly, however. The latter tend nowadays to rely heavily on "multi-parameter" radars in addition to instrumented aircraft. The radars of choice are one or more Doppler, dual-frequency, differential reflectivity, or polarization radars for tracking air motions and identifying precipitation particles, sizes, motions, and concentrations in individual clouds or cloud systems.

Some Current Topics

The world climate is frequently cited as the motivation for research on the relationship between the microphysical characteristics (the number and size of droplets or ice crystals) and radiative properties of widespread cloud types such as cirrus and lower level stratiform clouds. Recent comparisons between aircraft-measured cloud microphysical characteristics and satellite-detected radiative properties of marine stratocumulus clouds at 3.7-μm wavelength have provided direct confirmation that higher cloud reflectance (brightness) is associated with smaller cloud droplets. A primary source of droplet size variations is differences in aerosol concentrations between continental and marine air masses. An interesting example of the effect of anthropogenic aerosol sources on cloud reflectance are so-called "ship tracks." These were first observed in satellite imagery when ship's emissions formed trails of visible clouds. However, they appear more frequently in satellite imagery as modifications to the brightness of existing stratus and stratocumulus clouds. It is becoming increasingly clear that the radiative properties of cirrus clouds are dominated by small (shorter than 20 μm) ice particles which are not detected by conventional instruments and which contribute little to the total particle mass in the clouds.

Another topic of current interest is entrainment – the turbulent mixing of drier air into the cloud from outside. It has been known for a long time that entrainment occurs in clouds, ever since aircraft measurements revealed that the liquid water content in clouds was less than would result from adiabatic cooling. There is no doubt that the microphysical structure of clouds is a consequence of entrainment. Current research on entrainment focuses on the following questions: (1) On what scale(s) does turbulent mixing of entrained air take place? and (2) What effect does entrainment have on the droplet size spectrum? Almost 10 years ago it was suggested that the mixing process may be sufficiently inhomogeneous to cause some volumes within the cloud to experience more droplet evaporation than others. Consequently, these parcels would undergo a greater reduction of droplet numbers and liquid water content (LWC) than others. It was theorized that when these diluted, low-LWC parcels ascended in the cloud, the fewer droplets would experience enhanced condensational growth because of reduced competition for the moisture. A favored few droplets could then grow larger than the 30-μm-radius threshold needed to initiate the process of rapid growth by coalescence. This theory has received widespread attention because it offered a possible explanation of how coalescence and rain are initiated in warm clouds. As reported at the conference, however, recent observations indicate that this mechanism may not play an important role in continental clouds. The reason for this is that continental clouds appear to exhibit a high degree of fine-scale mixing, which produces diluted parcels with typical dimensions of 1 to 10 meters. Parcels of this small size are likely to be destroyed through further mixing before they can ascend distances of 100 meters or so necessary to allow sufficient condensational growth.

A type of severe weather cloud system that has been drawing interest in the 1980's is the vast thunderstorm system known as the mesoscale convective complex (MCC). These long-lived (12-36 hour) storms have gradually been recognized from satellite imagery as a rather common summertime phenomenon in certain geographic regions. In the US they occur nearly exclusively east of the Rocky Mountains and can cover an area as large as an entire state. Although MCC in some localities may generate tornadoes in addition to vigorous thunderstorm activity, a principal characteristic is the long-lasting, heavy rainfall from a widespread, trailing stratiform region of the complex. Some aspects currently under investigation are:

- The initiation and maintenance mechanisms for these vast complexes, including the widespread precipitation
- The structure and organization of the complexes

- The movement of air and high-altitude precipitation within the complex.

These MCC are of interest mainly to US researchers. The nearest equivalent in Europe and Asia is the "supercell" thunderstorm where hail damage is the greatest concern.

Acid rain is a current environmental issue along with the general topic of cloud chemistry: acid precipitation drew 21 papers in two sessions. Half of these were by US and Canadian authors. European interest was very modest, with the University of Manchester Institute of Science and Technology (UMIST) contributing the most (i.e., three) papers. UMIST and others reported measurements from instrumented mountain slopes in England, Germany, Switzerland, and Sweden. These sites allow the chemical comparison of precipitation at the base with droplets in the clouds intercepted up the slope. Scavenging of gases and particulate aerosols by droplets in the cloud and by precipitation below the cloud can thus be differentiated.

Four years ago this same conference appended a special day-long session for papers related to the "nuclear winter" theme. This year there was no mention of the topic, although some related cloud physics research has been going on in the US.

Classic Problems

In addition to the above topics, many of the classic cloud physics problems still exist to some extent. These include:

- The initiation of ice particle growth in cold clouds: how, where, and when will ice particles form?
- The mechanisms of rain formation in warm clouds where no ice particles exist to start the process. A few larger than normal cloud droplets appear to be necessary to start raindrop growth by coalescence; but how, where, and when are these larger droplets generated?
- The electrification of clouds. Sir John Mason, the eminent cloud physicist from the University of Oxford, lamented that after 30 or 40 years of cloud studies, there is still no definitive proof or disproof of a connection between electrification and the development of precipitation. Diverse evidence does indicate, however, that lightning will not develop in a totally liquid cloud nor in a totally glaciated cloud. For some reason, both ice particles and liquid drops appear to be necessary.

The Most Active Countries

The European and Asian countries contributing the most papers at the conference were:

- West Germany, 26 papers, mostly from the German Aerospace Research Establishment (DFVLR) in Oberpfaffenhofen (near Munich), and from 10 other institutions – universities, etc.
- Japan, 21 papers, mostly from Hokkaido University in Sapporo, the Meteorological Research Institute in Tsukuba, and from six other universities, etc.
- The Soviet Union, 19 papers from 10 institutes or government agencies (no universities!).
- The UK, 16 papers, mostly from UMIST and the Meteorological Office in Bracknell.
- France, 15 papers, mostly from the Laboratoire Associe de Meteorologie Physique (LAMP) in Aubiere or Clermont-Ferrand, and from the Meteorologie Nationale in Toulouse and Magny les Hameaux.
- China (PRC), 14 papers, mostly from the Institute of Atmospheric Physics in Beijing, and from five other institutes or universities.
- Other countries (except the US and Canada) contributed four or fewer papers each.

The contributions from DFVLR are from the Institut für Physik der Atmosphere or the Institut für HF-Technik. The former is concerned mainly with aircraft observations of cloud turbulence, convection, and microphysics, including applications to aircraft icing concerns. The HF-Technik group is involved with applying their new coherent, polarimetric, Doppler C-band radar to study precipitation rates and size spectra in large, convective cloud systems.

In the UK, UMIST has been concerned with the still-perplexing problem of warm rain initiation. Some work has also been done on the solution chemistry of cloud droplet nuclei dissolved in the cloud droplets. A polarization radar has also been used to study raindrop shape distortions. The work by the Meteorological Office in Bracknell includes: (1) aircraft studies of ice particle development in maritime and cirrus clouds, (2) aircraft and two-dimensional numerical modeling studies of radiatively driven convection in the top of boundary layer clouds, and (3) the response and accuracy of airborne temperature and particle sizing probes.

In France, the research at LAMP has relied heavily on major field projects with radar and instrumented aircraft measurements of frontal and large convective clouds. Studies include ice particle multiplication and riming growth of graupel. They have also contributed heavily to documenting microphysical variables in aircraft icing conditions and to the study of ice accretion on aircraft and land-based structures. They have been particularly productive in analyzing the response and accuracy of airborne particle sizing probes. The LAMP researchers report that they are now turning their attention to cirrus cloud studies, the motivation being the general problem of the influence of cloud cover on radiation transport and climate.

The French Météorologie Nationale has been studying a variety of phenomena including: (1) entrainment

and mixing processes in clouds and the resultant effects on droplet growth, (2) rain development in warm clouds, and (3) particle sizing instruments. In common with LAMP, the research again relies heavily on major, cooperative field experiments with Doppler radars and instrumented aircraft.

The papers from the USSR covered a wide range of topics. However, about half of the papers dealt with one of three subjects: (1) hailstorm development and hail formation, (2) electrical effects on hydrometeor development and (3) cirrus clouds. It is interesting that only two of the 19 contributions from the USSR could be classified as a numerical modeling study. Neither of these two involved the use of two- or three-dimensional cloud models to simulate the dynamical and microphysical evolution of convective clouds. It is not known to what extent the papers presented at the conference are representative of cloud physics research in the USSR. One can speculate that the apparently small effort in cloud modeling is due to the limited availability of high-speed computers for cloud physics research.

In China, cloud physics research is mainly concerned with microphysical processes and rain formation in cumuliform and stratiform clouds. There is also some interest in radiation fogs. Acid rain is obviously a problem of concern in China, as two papers described numerical simulations of the acidification of precipitation. A surprising eight of the 14 papers from China were numerical modeling studies, indicating that a strong emphasis is placed on this approach. Most of the modeling is being done at the Institute of Atmospheric Physics of the Chinese Academy of Science in Beijing. Some modeling is also being done in the Department of Geophysics, Peking University. Cloud seeding experiments and other field programs are conducted by numerous institutes around the country.

11/29/88

REPORTS ON EUROPEAN SCIENCE AND TECHNOLOGY FROM OTHER COMMANDS

Reports

Information on each of the reports listed below was furnished by the activity identified by the abbreviations for that office. Report numbers are given in brackets after the titles. Requests for copies of or information about the reports should be addressed to the appropriate office:

USARDSG – US Army Research Development and Standardization Group, Box 15/65, FPO New York, 09510-1500

EOARD – European Office of Aerospace Research and Development, Box 14, FPO, New York 09510

Biological Sciences

Olfactory Receptor Proteins [send inquiries to USARDSG].

While several components of the molecular olfactory mechanism distal to the receptors have been extensively studied, the protein receptors themselves remain elusive. Their understanding constitutes a major challenge for olfactory research. Investigations underway in the Department of Membrane Research at the Weizmann Institute, Rehovot, Israel, center on the identification, isolation and molecular cloning of olfactory receptor proteins. The research relies strongly on the knowledge of postreceptor components which was obtained during the last 3 years in the laboratory of the principal investigator, Professor Doron Lancet. Such information includes the identification and study of functional membrane proteins in olfactory cilia, namely olfactory GTP-binding protein (G-protein), odorant-sensitive adenylate cyclase, and the cilia-specific glycoproteins gp95 and gp56, which are prominent olfactory receptor candidates discovered by Professor Lancet. Investigations in this area involve a number of strategies. Besides utilizing antibodies in attempts to more fully characterize the role of specific proteins of olfactory epithelium, cDNA library screening is used with oligonucleotides synthesized according to the amino acid sequence of peptide fragments where these can be obtained. Also included are studies of olfactory-specific cytochrome P450 enzymes, which may participate in olfaction. A new species of the latter has been successfully cloned.

In studies based on the proposed homology between olfactory receptors and other G-protein-coupled receptors, Lancet's group has isolated several rat olfactory-eptithelial cDNA clones by using two new oligonucleotides synthesized according to a region of high homology among different B-adrenergic receptors, muscarinic acetylcholine receptors and visual opsins. This region is located in the second of the seven transmembrane domains in these G-protein-coupled receptors. In addition, they have synthesized an oligonucleotide based on a receptor region suggested to participate in the activation of Gs, in the cytoplasmic loop between transmembrane regions 5 and 6. This probe is used in parallel as a means of identifying cDNA clones coding for G-protein-activating receptors.

In receptor phosphorylation studies, they have defined a set of conditions, which include reconstitution of ciliary proteins into phospholipid vesicles, as well as pretreatment of the cilia with mild denaturants that inhibit endogenous kinases, but spare transmembrane proteins. These conditions allow the observation of a clear-cut B-adrenergic receptor kinase

phosphorylation signal. A prominent polypeptide substrate is apparent under such conditions. Such substrate may be the long sought olfactory receptor protein.

Models of Cerebral-Body Perfusion and Cerebral Chemical Transport, by Professor Jacob Bear, The Technion, Institute of Technology, Haifa, Israel. (65 pp) [EOARD-TR-88-05]

A sequence of models is constructed to simulate the movement of fluids and chemicals in the cerebrovascular system. One model simulates the nonsteady response of perfusion in various sections of the brain. In a second model, certain relevant parts of the body are added to form a single brain-body model. A third model simulates the transport of selected chemical components through the cerebrovascular system. Predictions derived from the brain model were shown to be well within the range of available clinical observations. The brain-body model describes the interaction between the cerebral, the cardiovascular, and the respiration systems. It is excited by expiration/inspiration fluxes and accounts for the effects of hydrostatic, environmental pressures, flight maneuvers with excessive (head to bottom) gravitation, acceleration, and resuscitation procedures. In simulating chemical processes in the brain, the model accounts for CO_2, HCO_3^- and H^+, as they are transported by perfusion and diffusion in the presence of chemical reactions. This model also focuses on the flow control between brain arteries and capillaries, due to changes in CO_2 concentration.

Chemistry

Probing Organic Molecules at Clay Surfaces [send inquiries to USARDSG].

Stationary and time-correlated fluorescence spectroscopy is a very sensitive tool to study adsorption at the surface of colloidal silica and clay suspensions. Particularly, single photon timing with picosecond resolution using global analysis of the decay data is a method of choice in studies conducted by Professor Frans de Schryver at the University of Leuven in Belgium. Several models describing the fluorescence decay have been developed, including the fractal concept. To investigate this phenomenon at clay surfaces, positively charged detergent-like pyrene derivatives were synthesized and adsorbed on the negatively charged surface:

$$Py\text{-}(CH_2)_n\text{-}N^+(CH_3)_3X^- \quad (1)$$

In particular the intermolecular excimer formation of (1) (n=3) on a clay surface gives interesting information on the adsorption process. Their observations, in agreement with other literature data, indicate a nonhomogenous distribution of the adsorbed detergent-like molecules on a clay surface in aqueous suspensions. The driving force for this nonhomogenous distribution is, to a certain extent, related to the distribution of the negative charges on the surface, but in aqueous suspensions the hydrophobic effect is predominant. Coadsorbed detergent molecules act as a dilutent and cause the excimer formation to diminish. The efficiency as dilutent was found to be dependent on the length and the structure of the detergent tail. It was found that the alkyl chain of the detergent must have a length which is the same or greater than the length of the probe molecules. This further corroborates the above observation of the importance of the hydrophobic effect as a driving force for cluster formation. In a clay suspension two different surfaces can be distinguished; the external and the interlamellar surface. It was found that excimer formation is different at both surfaces. At the interlamellar surface a less stable excimer is formed.

In combination with viscosity and light-scattering measurements, the excimer formation can also be used to study the stability of clay suspensions. It was found that even in very diluted clay suspensions the platelets aggregate, and that this aggregation is favored by the adsorption of a small amount of detergent-like molecules. The study at different loadings of probe and detergent indicates a reorganization of the adsorbed molecules on the clay surface at a given concentration (loading = 10 percent). This reorganization results probably in the formation of hemi- or admicelles, a known phenomenon in the adsorption of detergents at a surface. This micellization process is only observed for detergents adsorbed at the external surface. Recently, a study of a photochemically initiated polymerization of detergents having a polymerizable function in the head group has been realized and the properties of the obtained colloidal suspension are being studied by fluorescence spectroscopy in combination with viscosity measurements and G.P.C.

In the study of silica particles a pyrene derivative has been covalently bound to the surface to avoid exchange phenomena. Adsorption of organic molecules as well as the mobility of the silica particles in suspension and the mechanism of flocculation are studied using fluorescence and fluorescence quenching.

French Scientist Collaboration with MTL [send inquiries to USARDSG].

This summer, the Chemistry Branch arranged for a French scientist, Dr. Claudine Noel, to visit, in collaboration with Dr. Robert Singler, the US Army Materials Technology Laboratory (MTL). While there, Dr. Noel held discussions with MTL staff and presented a seminar on her research underway at the CNRS Laboratory of Physical Chemistry in Paris. During her talk entitled "Characterization of Liquid Crystalline Side-Chain Polymers," she reviewed recent results on characterization of a number of these polymers prepared for possible exploitation as ferroelectric materials and applications in general areas of optical devices and, more specifically, in wave guide devices which utilize nonlinear optical properties.

The polymers are methacrylate-based polymers with flexible spacers based on repeating methylene and ethylene oxide segments. The mesogens are aromatic esters, stilbenes, and biphenyl derivatives. Tailing groups include long chain alkyl substituents and cyano groups.

The influence of the chemical structure on the thermal stability range and the nature of the mesophases were discussed. An attempt was made to integrate the information available for the thermal data, textural phenomena, and x-ray diffraction patterns in a discussion of the specific features of the mesophases exhibited by these polymers. Molecular models consistent with the x-ray patterns were presented and the arrangement and association of the polymers in the various mesomorphic states were illustrated and discussed.

Improved Adhesion for Polymer Composite Tapes [send inquiries to USARDSG].

Professor A.J. Kinloch, Imperial College-London, recently participated in the US Army Materials Technology Laboratory's Sagamore Materials Con-

ference Series held in New England. Each year about one hundred researchers, in-house and external to various Army laboratories, are gathered to focus on one high-priority materials technology problem such as this year's conference on adhesives and adhesive bonding. Kinloch's research has shown that significant improvement in bond strength can be achieved by treating the surfaces to be bonded with a corona discharge. After treating the composite, the crack ran either in the adhesive in a cohesive mode or in the composite in an interlaminate mode. Failure stresses of the composites have been quantified using butt joints and these values have been compared with finite element analysis (FEA) predictions. There was good correlation between the two sets of data – i.e., when the stress in the composite predicted from FEA was higher than the measured failure stress from a butt joint experiment, the crack propagated in the composite, and vice versa. These new results were presented at the meeting and are available through the fifth periodic report just issued.

Physical Chemistry Research at Universities of Leeds and York, by LTC C. Dymek, EOARD. (20 pp) [EOARD-LR-88-06-I]

The Universities at Leeds and York both have high-quality research programs in physical chemistry led by inventive and productive scientists. They have very good to excellent facilities and there appear to be good opportunities for interdisciplinary programs. The areas most likely to be of interest to the Air Force at York included nonempirical MO calculations on small polyatomic molecules at high levels of rotational and vibrational excitation (Professor Sutcliffe) and overtone-induced photodissociation studies of proton – and possibly H-atom – transfer in condensed phase (Dr. Goodall). At Leeds the most likely source of a proposal is the work of Drs. Boden and Bushby in polymer formation by induced linking of liquid crystal molecules in the ordered phase. Other ongoing work is in evaluation of kinetic data and in combustion and explosion chemistry.

1988 European Computational Chemistry Workshop at Oxford University, by LTC C. Dymek, EOARD. (2 pp) [EOARD-LR-88-060]

This annual workshop was attended by scientists from nine Western European countries. The latest capabilities of a number of computational methods, including ab initio, molecular mechanics, semiempirical, and data base searching were presented in lecture and laboratory sessions. USAF was represented by Dr. Jimmy Steward (USAFA/FJSRL), who presented the MOPAC workshop. Plans to improve the resources provided by the USAFA/FJSRL computational chemistry center to other AF Labs emerged from the workshop. These include implementation of more useful database searching programs for organic reactions and structures and development of capabilities to construct MOPAC data files for large molecular systems using graphics software.

Research Work at University College, Dublin, by LTC LaRell Smith, EOARD. (8 pp) [EOARD-LR-88-057]

The Chemistry Department at University College, Dublin has work in a number of areas which overlap with Air Force interests. Dr. Kenneth Glass is an acknowledged expert in the interpretation of IR and Raman spectra for transition metal complexes, particularly those of hydrazine and methylhydrazine. Dr. R. O'Neil has initiated a program to follow neurochemical processes using electrochemical techniques, and Professor David Brown has a strong program in calculations chemistry for predicting reaction profiles for transition metal complexes.
Environmental Sciences

Earth Sciences

Evaluation of CPT and DMT in Crushable and Silty Sands [send inquiries to USARDSG].

Engineers have been using empirically the principle of a penetration means to make strength assessments since the beginning of this century. The geotechnical knowledge since 1928 has spiralled in theoretical and applied characterization of *in situ* soil properties. However, because of the inherent problem of recovering *in situ* undisturbed granular material samples for testing, the determination of the properties of *in situ* granular material have been elusive. Professor Jamiolkowski (Torino Technical Institute) and Dr. Eng. Roberto Bellotti (National Electricity Board of Italy [EWEL], Hydraulic and Civil Engineering Research Center, Milan, Italy) have developed in the last decade innovative approaches to determining the *in situ* material, requiring heavy capital laboratory testing equipment, e.g., large Callibration Chambers that are capable of replicating *in situ* conditions. This research is linked with a WES Geotechnical Laboratory work unit in characterizing existing dam foundations on silty sands that might be subjected to dynamic loads which could cause liquification. The Torino Technical Institute in conjunction with ENEL, is the supreme center for investigations of this nature. Dr. Bellotti has been awarded a contract for the evaluation of the correlation between the engineering parameters of crushable sands and the results of Static Cone Penetrometer (CPT) and Marchetti's Flat Dilatometer (DMT) to assess the stress-strain and strength characteristics of crushable materials like glauconite and calcareous sands. The CPT will be used to look at these characteristics and a limited number of DMT's will be performed with the aim of investigating the possibility of assessing the coefficient of earth pressure at rest. The work will be performed on test sands using a glauconite sand and two course calcareous sands. The main part of the work will be the CPT's and DMT's performed in the Calibration Chamber (CC). Both dry and water- saturated specimens will be tested. The CC tests will be supported by a certain number of small-scale laboratory tests in order to obtain an adequate stress-strain and strength characterization of the test sands. The experimental data resulting from the tests will be stored in a data bank created for the purpose of making the data reduction and interpretation easier and supported by a number of statistical subroutines.

Environmental Sciences

On-Line Point Positioning with Single-Frame Camera Data [send inquiries to USARDSG].

The U.S. Army Engineer Topographic Laboratories' have a program for enhanced capabilities to "look-deep/shoot-deep." In the future, near-real-time imagery from a broad suite of reconnaissance sensors will be transmitted to ground forces. Ground control to support on-line point position will be available in the 1990's from the Digital

Point Positioning Data Base (DPPDB). Improved and analytical solutions for on-line point positioning are needed to develop simpler, more robust algorithms for use in future field systems, which will have a direct impact on critical operational capabilities.

Professor Dr. A. Gruen of the Institute of Geodesy and Photogrammetry, ETH-Hoenggerberg, Zurich, Switzerland, has been awarded a contract to develop a fast, reliable, and precise online triangulation procedure on analytical plotters. Developing a data processing concept for online high-accuracy point positioning single-frame camera systems includes (1) investigation of at least two different sequential algorithms, which were proposed recently within the mapping community for online photogrammetic triangulation (Triangular Factor Update, Givens Transformational); (2) development of suitable rejection procedures for blunders and nondeterminable systematic error components in sequential self-calibrating systems; and (3) a technique of "Analytical Point Transfer," which can efficiently be used on analytical plotters. This new measurement procedure would work even without distinctive natural, signalized, or artificially marked ("pugged") tie points.

International Association of Engineering Geology (I.A.E.G.) [send inquiries to USARDSG].

The International Association of Engineering Geology held a symposium, September 19-23, 1988, in Athens, Greece, which focused on the preservation and protection of ancient works, monuments, and historical sites. Accelerated deterioration of ancient structures in recent years, associated with the rapid development of modern societies, has led to an increase in research work and practical studies towards the conservation of national monuments.

This symposium offered the opportunity of acquiring the experience gained thus far throughout the world in this field. Many interdisciplinary subjects were covered, such as engineering geology, ancient works, monuments and historical sites, soil and rock mechanics, foundation engineering, structural geology, geomorphology, geophysics, and seismology. Approximately 160 papers were presented and published in three volumes of the Proceedings. A fourth postsymposium volume, containing general reports, written discussions, short notes, and late papers will also be prepared. Selected papers will be published in a special issue of the journal *Environmental Geology and Water Sciences*, and selected papers are also planned to be published in *Geoarchaeology*. Approximately 250 scientists participated in the symposium. Mr. Comati (USARDSG-UK) concentrated on topics of interest to the US Army such as geotechnical protection of historical retaining walls and foundations, underpinning of the scoured piers of bridges, analysis of disorders and remedies affecting ancient structures, and seismology, which are of concern to the Environmental Laboratory of the Waterways Experiment Station.

Fluid Mechanics

Experimental Investigation of Retarded Unsteady Turbulent Boundary Layers [send inquiries to USARDSG].

Unsteady turbulent boundary layers are of great practical importance. Some effects of forced unsteadiness, as on lift and stall of an airfoil, are well known but cannot be explained because the present-day grasp of the basic physics of these flows is quite limited.

A coherent picture of the behavior and interactions – or the absence of interactions – between the mean, periodic, and turbulent flow field in zero pressure-gradient boundary layers starts to emerge from various experimental observations despite some disagreements about interpretations of available data or even about the data itself. The picture is much more confused for unsteady boundary layers subjected to adverse pressure gradients which are more complex and have been studied in far fewer investigations than the flat plage or channel flows. They are, moreover, also of greater practical significance.

The aim of this research by Mr. Gilbert Binder of the Institute de Mécanique de Grenoble, France, is to investigate two families of unsteady turbulent boundary layers in mean adverse pressure gradients, one in a moderate gradient without separation and one in a strong gradient leading to separation. Moreover, since the bursting process is the key phenomenon in the generation of wall turbulence, another objective is to investigate its response to periodic unsteadiness and more generally the response of the turbulent structure.

The research is being carried out in a water tunnel which has the capability of generating forced oscillations over a wide range of frequencies and amplitudes and in which continuous adjustment of the pressure gradient can be made. Measurements of velocity and wall shear stress are made with laser-Doppler and hot-film anemometers. Measurements can be made down to the viscous sublayer, a unique feature among existing unsteady flow facilities.

During the initial phase of this work – under the cost-sharing portion of the contract – the flow loop was constructed and the apparatus needed to perform the experiments was constructed, evaluated and redesigned as needed. For example, the water tunnel walls were made easier to move and control so adverse pressure gradient could be changed more easily, quickly, and precisely and the apparatus for pulsating the flow was modified, making the pulsations more precisely controlled and repeatable. Improvements in instrumentation were also made as preliminary data and valuable operating experience were compiled, including: automatic, preprogramed control of the location of simultaneous hot-film and LDA measurements in the free stream, automatic calibration and zeroing of all hot-film gages, and the addition of hot-film gages. Software for the automatic positioning control and for real-time data acquisition and reduction were also performed.

The research has first been focused on the response of the turbulent structure and in particular on the bursting phenomenon. In order to have a solid basis for comparison, the investigation was first conducted in zero pressure gradient flow. Simultaneous measurements of velocity and shear stress have been recorded for ten different oscillation conditions. It has been shown that the bursting process is strongly modulated by the imposed oscillations whether the detection is based on the sweeps as with the VITA scheme or on the ejections as with the u'-level scheme even though the thresholds are modulated proportionately with the instantaneous phase-averaged value of the turbulent intensity. Interestingly, the

conditionally averaged u'-signals of the sweeps have considerably stronger cyclic modulation than the turbulent intensity itself.

Another remarkable observation is that the skewness of the time derivative du'/dt which is an intrinsic feature of turbulence related to vortex stretching and the energy cascade from large- to small-scale structures is also modulated. The imposed oscillatory motion is thus felt through the whole spectrum and affects all the turbulent mechanisms.

Instantaneous Flow Field Measurements in the Boundary Layer and the Near Wake of an Oscillating Airfoil [send inquiries to USARDSG].

The boundary layer over a sinusoidally oscillating airfoil and the near wake region have been experimentally investigated by Professor Ch. Hirsch of the Vrije Universiteit Brussels, Belgium. The objectives of this research at this stage were (1) to study the formation of the leading edge separation bubble and development of leading edge stall and (2) to investigate the Kutta-condition and development of the wake during deep stall. In general, these investigations will contribute to the data base of experimental results used to verify computed results. (Toward that end, a full set of data has been sent to Dr. L. Carr at AVSCOM, NASA Ames Research Center.)

The mean velocity components and the Reynold stress tensor were measured with a slanted single-sensor hot-wire rotating about its axis. The method of data analysis used in those experiments, capable of detecting flow reversal, was developed at the Fluid Mechanics Department of the university. The mean and the rms values of the hot-wire output were separated by ensemble averaging over 100 cycles of oscillations, and the data were recorded for 542 timesteps in each cycle. Each of the measured quantities resulted from the outputs at 19 angular positions of the rotating hot-wire, out of a total of 48 angular positions considered. To the best or our knowledge this is the only investigation of unsteady flow over a pitching airfoil in which the velocity components and the Reynolds stress tensor have been measured.

For this stage of the program the following two test cases were investigated:

- Airfoil operating with leading edge stall
- Airfoil operating with a leading edge separation bubble.

The airfoil used was a 60-cm chord, 94-cm span NACA 0012 airfoil section oscillating at 1.84 Hz. The air velocity was maintained at a nominal speed of 11.2 m/s to give a chord Reynolds number of 300,000 and reduced frequency of 0.31.

Figures 1 and 2 [in the original USARDSG document] show the measured mean velocity vectors around the airfoil at various angles of incidence while the airfoil was oscillating between 10-20 degrees and 8-18 degrees, respectively. These are examples of the airfoil operating with deep stall. Figure 1 clearly shows the trailing edge separation, the formation of a vortex near the leading edge and this vortex rolling over the suction surface towards the trailing edge during a period of oscillation. Figure 2 shows trailing edge separation just before formation of the leading edge vortex, the leading edge vortex rolling over the trailing edge, and formation of a trailing edge vortex just after the leading edge vortex rolls over the trailing edge.

Figure 3 [also from the Army Document] shows the averaged hot-wire traces and their rms values over two cycles taken near the leading edge of the airfoil, during 5 to 15 degrees of oscillation. The sudden change of output of the hot-wire indicates the presence of the separation point. The separation is accompanied by a sharp rise in the rms output. The separation bubble extends from about 30 mm to 60 mm from the leading edge along the surface when the angle of incidence is 15 degrees. Measurements are being conducted to survey the flow at this oscillation which is the same as case 2 mentioned above.

Materials Science

Residual Strain Measurement in Uranium [send inquiries to USARDSG].

Using the UK Synchrotron Radiation Source, SAS, with a 5-Tesla wiggler, Professor W.F. Sherman and Dr. D. Hauserman at Kings College, London, have shown in their final report that energy dispersive x-ray diffraction, EDXRD, and the $\sin^2 u$ method of residual stress measurement can be successfully combined to measure lattice strains of less than 1 part in 10,000 with an accuracy of 50 percent or better. Because of the high absorption coefficient of uranium, measurements could not be made in the bulk of the material with the range of x-ray energies available. Hence, they had to be made in reflection from a thin layer of the surface containing oxide. Further, as uranium has an orthorhombic structure, ideal experimental parameters are high-energy synchrotron radiation and low angles of diffraction in order to achieve optimum resolution. In reflection geometry these conditions limit the range of tilt, and hence lower the accuracy of the calculation of the residual stress. This also reduces the depth of penetration further so that in the work reported here, the maximum value of the effective penetration thickness was approximately 5 μm at 50 keV. Faced with these limitations, the simplest form of analysis was chosen: the ($\sin^2 u$) method with the assumptions of a single-axis stress state and of no stress component in the direction of the surface normal. The probable anisotropy of the elastic properties within the individual crystallites resulting from the interaction between the measured crystal strains and the surface stress were ignored; hence the elastic constants predicted by isotropic elasticity theory from the bulk modulus were used. [The data used to calculate the residual stress are shown in the original USARDSG document.]

All restrictions become less severe as the atomic number of the materials are reduced. Stress measurements are currently being made on iron using synchrotron radiation from SRS wiggler in transmission geometry and in samples up to 15 mm thick. Such measurements could also be made using a high-voltage generator, but with samples only a few millimeters thick to compensate for the large reduction in the intensity of the radiation. Detailed stress analyses which have only been performed on sample surfaces using the angle scanning mode could then be made inside materials using transmission geometry at a fixed angle of diffraction. This was the final report on Contract DAJA45-86-M-0507 and is available through NTIS. The results of this investigation were presented in a Seminar at the Materials Technology Laboratory by Professor Weiss of Kings College in September 1988.

Mathematics

Modelling Combat [send inquiries to USARDSG].

The draft final report of a USARDSG-UK research contract funded by the TRADOC Analysis Command (TRAC) has been completed. The Principal Investigator on this contract, entitled "Modelling Combat as a Series of Minibattle," was Michael R. Bathe of the Royal Military College of Science (RMCS). This work was also supported by the Directorate of Science (Land) of the UK Ministry of Defence.

This research was concerned with investigating the possibility of decomposing a main battle into a number of smaller engagements, or minibattles. The main sources of data were armour/anti-armour combat trials held in Europe and the US. Results of the data analysis are presented together with conclusions as to how these might be used in the formulation of a network combat model. Various network and attrition methodologies were investigated with a view to finding appropriate methods for incorporation in such a model. Finally, the development of a prototype combat model was discussed.

Research on Statistical Inference of Stochastic Processes [send inquiries to USARDSG].

Dr. G.R. Andersen, Chief of the ERO Mathematics and Physics Branch, met with mathematical statisticians at Universities in Denmark and Norway. These scientists, Per Kragh Andersen, Statistical Research Unit, and Martin Jacobson, Institute of Mathematical Statistics of the University of Copenhagen and Odd Aalen, Section of Medical Statistics, and Ornulf Borgan, Institute of Mathematics of the University of Oslo, are part of a group, primarily from the Scandinavian countries, Finland, and the Netherlands, who have worked together to produce a theory of inference for counting processes. Their aim has been to develop statistical models for life history data based on counting processes (e.g., survival analysis or failure time analysis). Although this subject has a long history, the 1975 thesis of Odd Aalen, obtained at the University of California at Berkeley, provided a fundamental breakthrough utilizing the then newly developing general theory of stochastic processes (semimartingales and stochastic integration) that resulted in a unified and general analytic framework based on counting processes in which censored failure time data could be studied. He also showed that classical failure models had the multiplicative intensity structure that he introduced. During the next 10 years his methods were taken up and utilized by the extremely talented group of scientists alluded to above in order to extend numerous methods from the survival analysis literature and to begin a rigorous and complete development of a theory of inference for statistical models based on multivariate counting process.

The discussion at the University of Copenhagen with Per Andersen provided numerous examples of the Statistical (Biometry) Research Unit's efforts to solve practical problems with these methods. In fact, it appeared that their interest in developing the theory was solely based on their need to solve difficult and unusual statistical problems. Recent problems considered by this group have resulted in papers in medical, actuarial, and reliability journals. On the life science end, they include a study of the mortality of insulin-dependent diabetics, psychiatric admissions related to abortion, and the occurrence of metastases of multiple sites after breast cancer.

Martin Jacobson's work is primarily mathematical, most recently providing, for example, conditions on censoring patterns which would allow the use of Kaplan-Meier estimator as an estimator of the survivor function for a failure time distribution, or in constructing necessary and sufficient conditions for the maximum likelihood estimator in certain exponential families to exist and be unique.

Borgan's work appears, as that of Per Andersen with whom he collaborates, to be highly motivated by practical problems. The discussion with Odd Aalen gave some indication as to how one person could have had such a profound effect on mathematical statistics in just a little over a decade. He has not been working specifically on counting processes for the last couple of years, but is now returning to this area. His recent work has centered on what he refers to as dynamic statistical models. There he seems to have had several goals. Having convinced most statisticians that life histories should be viewed as stochastic processes and so causing them to leave the arena of independent random variables, he is concerned with the way they model these processes. The most commonly used dynamical model is a Markov process, but the Markov assumption seldom holds in practical statistical problems. Aalen argues convincingly that for statistical purposes the Markov assumption may be discarded and the more general theory of semimartingales used as a model for dynamical statistical systems. From this point he makes the obvious intuitive connection between causality and dynamic models and proceeds to introduce the notion of "local dependence" from which he obtains a rigorous way to describe one process being a "cause" of another without the converse being true.

Since a counting process is a special case of a semimartingale, recommending a semimartingale as the correct formulation for a dynamical statistical model is a natural and straightforward generalization of his earlier work. The important contribution here is his definition that a process $Y=(Y(t),\ t\ 0)$ is "locally independent" of a process $X=(X(t),\ t\ 0)$. He does this by first placing an additional restriction on the semimartingale representation of Y and X, namely, that the innovations portions of their representations be "orthogonal." This is almost no restriction since, intuitively, they would not be independent if the innovations of one process influenced the innovations of the other. Then he defines Y to be "locally independent" of X over some time interval by requiring the "predictable" part of the semimartingale representation of Y as a function only of the historical behavior of Y over that time interval. This work has been brought to the attention of scientists at the Walter Reed Army Hospital, the US Army Human Engineering Laboratory, and the Center for Night Vision and Electro-optics.

New Target Tracking Algorithms, by Dr. V.L. Donlan, EOARD. (4 pp) [EOARD-LR-88-69]

Stephen Blake of Analytic Associates in Gwent, Wales, has recently developed several new target tracking algorithms based on the processing of real, noisy, grey-scale imagery. In work completed in 1987, he derived the equations for a recursive target tracking algorithm that is correct to second order in the target-image coordinate space. In work completed in the spring of 1988, Blake developed a modified algorithm that accounts for unpredictable target dynamics.

More recently, he has reformulated the problem as a system of ordinary differential equations whose solution is exact to all orders of the coordinates. These new algorithms were developed using the mathematics of differential geometry and the concept of Lie dragging and are substantial improvements over commonly used heuristic methods of extracting target state information from noisy images.

Physics

Collisional Dynamics of Interacting Supersonic Molecular and Atomic Beams, by Dr. S.S. Lazdinis, EOARD. (4 pp) [EOARD-LR-88-63]

Professor K. Bergmann of the University of Kaiserslautern in West Germany is an expert in the development and application of new laser-based molecular beam techniques to study the collisional dynamics of interacting supersonic molecular and atomic beams. He possesses a unique experimental capability which employs an optically pumped molecular beam laser to generate supersonic beams consisting of dimers in preselected rotational and vibrational energy states and having specified values of angular momentum. His research dealing with the collisional dynamics of Na_2 with the rare gases He, Ne, and Ar is described.

Culham Laboratory, by Dr. V.L. Donlan, EOARD. (3 pp) [EOARD-LR-88-66]

Culham Laboratory is the UK AEA Center for fusion and plasma physics research. It is the site for the Joint European Torus. Recently, the laboratory has begun to diversify, applying its expertise to nonfusion research, such as neutral particle beam research for SDI, ion beams for spacecraft thrusters and propulsion, semiconductor processing, and industrial lasers. Current Culham Laboratory programs in these and other areas are briefly described in this report.

Research Work at Dublin Institute for Advanced Studies, by LTC LaRell Smith, EOARD. (10 pp) [EOARD-LR-88-058]

The Dublin Institute for Advanced Studies Cosmic Rays Section is one of the premier organizations in the world doing research in heavy cosmic ray abundance. They have one of the major experiments on the Long Duration Exposure Facility, which was launched from the Space Shuttle in 1984. They have numerous other experiments to define the spectrum of cosmic rays outside the earth's atmosphere as well as doing fundamental research on detection techniques for heavy cosmic rays—particularly the "lexan" technique which uses special polymer materials to detect ionizing radiation. This report gives some general details about the institute as well as describing the Cosmic Ray Section's work in more detail.

Semiconductors

Semiconductor Conference [send inquiries to USARDSG].

Dr. J. Zavada from the European Research Office attended the 19th International Conference on the Physics of Semiconductors (ICPS), which was held in Warsaw, Poland, from 15-19 August 1988. It was organized by the Institute of Physics, the Polish Academy of Sciences, Warsaw University, and the High Pressure Institute of Poland. The ICPS is a biennial meeting that normally attracts about a thousand participants. Since the present meeting was held in an Eastern Block country, American attendance was much lower than at previous sessions. There was, however, a larger than normal number of attendees from the Soviet Union and East Germany. Total number of attendees at the present meeting was between 800 to 1000.

The program consisted of four plenary session talks, 27 invited papers, 144 contributed papers, and 245 poster presentations. Of the plenary talks, three were by US scientists from private industry, and one by a Soviet scientist. Of the 27 invited papers, seven were from the US, 11 from the EEC, and six from the Eastern Bloc. So even though the number of US attendees was lower than in previous years, there was still a substantial US participation. In general, the plenary talks and the invited papers were of a review nature and represented the results of high-quality research.

The contributed papers at ICPS covered a wide range of topics in the area of solid-state semiconductors. Certain areas received particular attention, such as properties of low-dimensional systems and semimagnetic compounds. The Polish scientists have a strong history of research relating to the II-VI semiconductors and they presented a number of very good papers at this meeting. Other topics that received considerable emphasis were quantum Hall effects, surfaces and interfaces, defects in semiconductors, and electron transport. There were two poster sessions on successive days which were well attended.

All sessions were held in the Palace of Culture and Science, which is a huge building that the Soviets constructed as a gift to the Polish people. The conference halls were very good and the sessions were conducted efficiently. A book of abstracts was presented to the participants and conference proceedings will be published.

The next ICPS meeting is planned to be held in Thessaloniki, Greece, during August 1990. Circulars are already being distributed advertising the meeting.

The Army is developing various solid-state electronic devices for use in planned weapon systems. Advances in the processing and characterization of semiconductor material and structures is critical to the successful development of these systems. This conference provided useful information relating to such topics. In particular, the sessions on dilute magnetic semiconductors have importance for future night vision devices and the presentations on quantum structures is important for high-speed computation.

Gallium Antimonide-Based Devices, by Dr. E. Davies, EOARD. (3 pp) [EOARD-LR-88-70]

Centre d'Electronique de Montpellier, France is a CNRS research facility which has a strong semiconductor capability based on the gallium antimonide material system. The Center grows its own GaSb crystals, which are then used as substrates for subsequent epitazial growth. Devices produced by MOCVD include mid-infrared photodetectors that are compatible with fluoride glass fibers.

THE EMBASSIES: TECHNOLOGY ROUNDUP

France

For further information on items from France, contact Dr. Allen Sessoms, Office of the Science Counselor, American Embassy, Paris, APO New York 09777-09200.

The Europe of Technology. According to a report prepared by experts of the French Ministry for Foreign Affairs, the situation with respect to European cooperation in technology development has greatly improved. The mobilization of Europe has stopped the technological decline that Europe feared 10 years ago. But this success is not complete. Compared with the US and Japan, Europe is no longer losing ground but does not seem to be able to make up for lost ground. Further, there still exist shortcomings that Europe has not yet been able to overcome.

The situation related to technological developments in Europe has improved, in the words of the French authors, in "a spectacular manner." But they emphasize in their report that the US and Japan also have increased their efforts, while new competitors, such as South Korea, are coming to the fore. Furthermore, the amelioration is limited to traditional technologies. Europe should be vigilant in other high tech sectors if it does not want to be left behind again. This is particularly true for biotechnologies and new materials.

The report points out that in two key sectors (data-processing and electronic components), the 1984-1987 period was particularly favorable for European companies. In 3 years, the turnover for data-processing of six major European manufacturers (Siemens, Bull, Olivetti, Nixdorf, ICL, and Philips) has doubled from $10 million to $20 million. During the same period, the turnover of the medium- to small-size American manufacturers did not increase and that of IBM increased by 6 percent. European manufacturers now number four among the top 15 world manufacturers instead of the two in 1984. With respect to electronic components, the authors of the report indicate that Thomson (French) and SGS (Italian) have formed a joint venture. Europe has therefore three major groups – SGS-Thomson, Siemens, and Philips – whose investment/turnover ratio is higher than that of their US competitors. This renovated European industry develops competitive products. To illustrate this point, the report cites as examples the mini-supercomputers of Parsys (Great-Britain) and Talmat (France) which are three times as rapid as those of US competitors. Another example is high-definition television. The report, however, emphasizes that few of these products have undergone the test of large-scale marketing.

In spite of these results, the report asserts that the European information technology industry ranks third and is not aggressive enough in certain areas. For example, in the optical fibers sector, Europe is behind when it used to be ahead.

The European programs ESPRIT, BRITE, RACE, and EUREKA have contributed to the integration of Europe by encouraging industries and research institutes to cooperate. However, the integration is far from being complete. The authors of the report indicate that European strategies are limited to precompetitive development and long-term projects because there exist large national corporations or monopolies. For instance, the RACE program is aimed at preparing the telecommunications of the next century. In the meantime, however, the Europeans will have developed seven different commutation switches and will not be united to confront Japanese competition on new terminals and US competition on value-added networks and private communication satellites.

The European integration process is slow. This may become detrimental to Europe because the US and Japan are establishing tighter links and thus benefit (rather than suffer) from the technological development of the new industrialized countries. It is true that Europe has increased its research efforts and reoriented them towards industry. However, both the US and Japan did the same and therefore have maintained their technological advantage. Likewise, the European Community has created incentives to encourage cooperation between university laboratories and industries, but such partnerships have developed to a greater extent in the US and Japan.

The authors point out that, in spite of these shortcomings, Europe has proven that it can react. The European Community, which dealt with the most urgent problems, concentrated its efforts on information and telecommunications technologies. The funds allocated to these sectors for the 1987-1991 period amount to 2.275 billion ECU's ($2.60 billion) against 220 million ECU's ($250 million) for new materials and 120 million ECU'S ($138 million) for biotechnologies. While the US, Japan, and South Korea are very active, Europe does not convey the impression that it wants to be the first to manufacture and sell new products on a large scale. And this, in spite of the fact that it has assets, among which is a powerful pharmaceutical industry with substantial research resources. According to the report, this industry is extremely careful. The new medical technologies do not correspond to the chemical know-how of large pharmaceutical corporations and may threaten the advantage they derive from traditional therapeutics. This attitude can only be damaging when the Japanese pharmaceutical industry is preparing its breakthrough into the world market with the help of biotechnologies.

French 1989 Civilian R&D Budget. In the 1989 civilian R&D Budget, the funds allocated to support industrial research and innovation have increased by over 40 percent, from F1.556 million ($259 million) last year to F2.196 million ($366 million) this year.

This augmentation results from various factors: (1) a 31.18 percent increase in the funds allocated to the research and technology fund for the EUREKA program (the purpose of the research and technology fund is to encourage technology transfer through financial incentives); (2) specific industrial programs in the area of biotechnologies, materials, and nutrition; (3) a 23.96 percent increase in the budget of Anvar (Agence Nationale de Valorisation de la Recherche-[the National agency for the exploitation of research]) which must contribute to the development of the technological potential of small and medium-size companies; (4) F200 million ($33 million) that the industry ministry will allocate for techno-

logies with multiple applications; and (5) the so-called "research tax credit" (Credit d'Impot Recherche) which will amount to F2 billion ($333 million) next year (against F1.6 billion [$267 million] in 1988) and will affect 4,000 companies. (The research tax credit is a tax measure which consists of deducting taxes by an amount equal to 50 percent of the yearly increase in R&D expenditure).

This increase makes good on election campaign promises made by President Mitterrand. He is a firm believer that only advances in the technological sector and enhanced tech transfer between laboratory and industry will allow France to hold its own in the single European Market. The French government has made progress in this area in the past several years. This budget, which was passed by the national assembly, bodes well for future efforts.

Research on New Materials. Approximately F4 billion (about $667 million) in public and private funding is currently spent in France on research on new materials each year. French Research Minister Curien in collaboration with the Industry Minister wants to boost research in this strategic sector. Curien emphasizes, however, that the main problem is not so much to develop new materials in laboratories but rather to encourage technology transfer to industry.

In order to mobilize researchers, engineers, and industrialists and in particular small to medium-size companies which are not involved enough in these techniques, Curien proposed three types of measures: (1) to further develop research on certain strategic technologies, such as high temperature superconductivity; (2) to improve the circulation of knowledge within the framework of the major technological programs (such as space and nuclear) which contribute to the development of new materials (carbon-carbon or ceramics) or to the modification of existing materials (orientation committees will be created, with the approval of the ministry of defense for some of them, within the framework of these major programs, to ensure the circulation of knowledge); and (3) to improve coordination within public agencies. An interministerial group called "Innovation, Circulation, Materials" is likely to be created in the near future. It will have to periodically check on the status of research and the circulation of results as well as submit each year a report on the progress made, the ways to apply research, and the priorities to be retained.

The Netherlands

For further information on items from the Netherlands, contact CDR Donald Dahl, US, Office of Defense Cooperation, American Embassy, APO New York 09159-5770.

The Netherlands' Energy Research Foundation (ECN). The objective of the ECN, located outside the seaside village of Petten, is energy research, including energy-related environmental research. The facility employs 923 people, and has a budget of g130 million (approximately $65 million). Of the money, about g80 million are spent on personnel. ECN receives g54 million in subsidies from the government, about g12 million in research contracts from the government, and g7 million in research contracts from the EC and g33 million guilders from contracts and services to third parties (this g33 million amount includes g20 million for running Petten's reactor for the EC). Foundations and other sources provide the remainder of ECN's budget. ECN has a five-member board of directors, which includes a chairman who works at ECN, and representatives from government (Ministry of Economic Affairs), the research community, industry, and education.

ECN's revenues from services and contracts have increased steadily over the past years. In 1983, ECN earned g44 million from services and contracts, out of a total budget of g117 million, while in 1988, non-grant revenues reached g78 million. During the same period, the proportion of ECN's resources devoted to nuclear energy research decreased markedly.

Nuclear Energy Research. Nuclear research at ECN concentrates on the following issues: safety of thermal reactors, storage of radioactive waste, advanced fission reactors, radiation hygiene, nuclear analyses, and fusion reactors. While the Chernobyl accident caused the government to rethink use of nuclear energy as a power source, ECN continues to do research in this area to provide the Dutch government with information concerning the safety of nuclear power stations beyond its frontiers. ECN has carried out two studies following Chernobyl, one on the possibility of similar accidents, and another on the consequences of such accidents. The first study, completed last year, showed that similar accidents can be excluded for new power stations. The second study is not yet finished.

Safe disposal of nuclear waste is also of major concern to ECN, which participates in an international storage experiment in ASSE in Germany. Canisters containing nuclear waste simulating radioactive matter and chemical waste will be stored in the abandoned salt mine in ASSE. Researchers will then study the influence of heating and radiation on the thermomechanical behavior of rock salt. In cooperation with CERN in Switzerland, ECN researchers are also studying the effects of nutrients on tissue in a project on radiation hygiene.

Superconductivity Research. ECN has also manufactured superconducting niobium-tin wires, and has participated in two projects in this area, including development of a conductor for toroidal magnet coils of the "next European torus" (NET) and contribution to a test installation for NET conductors. ECN scientists presented papers on this topic at the 10th International Conference on Magnet Technology in Boston in September 1987.

Fossil Energy Research. In the area of fossil energy research, ECN concentrates its efforts on developing environmentally acceptable and efficient conversion techniques. ECN is studying fuel cells, primarily the molten carbonate cell, catalytic combustion of natural gas, coal gasification, fundamental coal combustion research, acidification, and water-silt-soil systems. ECN estimates that its fuel cell research will be on par with US and Japanese efforts in 1992. At present, its molten carbonate fuel cells have a 60 percent efficiency.

Renewable/Wind Energy Research. Given the Dutch climate, ECN's research efforts in renewable energies focus on wind rather that solar power. The goals of ECN are to make wind energy cheaper and more reliable in operation. Government policy in encouraging the use of wind power is based on environmental considerations, and on political concern which promotes the diversification of energy sources.

To this end, ECN tests and licenses windmills under a government subsidy program. The government provides subsidies to qualified Dutch windmill manu-

facturers, and to users in the Netherlands of approved windmills. There are 22 manufacturers of wind turbines in the Netherlands.) ECN tests and approves windmills for user subsidies regardless of country of origin and tests Dutch-manufactured windmills for producer subsidies. The quality certificates issued by ECN attest the safety, energy production, and noise emission of the particular windmill. In terms of costs, ECN estimated that until both oil prices and the value of the US dollar fell, the cost of wind energy in the Netherlands was only 20 percent more expensive than conventional power. However these two developments have again widened the cost structure. Nevertheless, the government hopes to be producing 1000 MW of wind-generated electrical current by the year 2000. As of September 1988, the Netherlands had 17.8 MW of installed windpower with an additional 9 MW under construction. For 1990, the government's goal is to have 100 to 150 MW of wind-generated energy.

Most of the wind turbines tested in the Netherlands are of small to medium size, but ECN also has one 300-KW horizontal shaft turbine with a rotor diameter of 25 meters. ECN is also testing autonomous wind diesel systems for use in supplying electrical energy in remote areas. ECN has developed a cheaper control system by which the power output of the wind turbine can be controlled so that gusts of wind do not cause a grid overload.

Research into High-Tech Ceramics. The ECN research efforts on ceramics also focuses on potential applications in energy, specifically energy conversion systems. ECN is attempting to develop new ceramic materials leading to new applications in membranes, fuel cells, fiber-reinforced strong ceramics, porous ceramic burner plates, and ceramic superconductors. The Dutch National Ceramic Workshop, established at ECN in 1986, concentrates on providing specimens of fine ceramics for research and development at ECN and for Dutch industry.

Dutch Aerospace Research. The Netherlands Agency for Aerospace Development (NIVR) and the Dutch National Aerospace Laboratory (NLR) are both active in aircraft development for the Dutch manufacturer Fokker, and in development of technology for space applications. NLR's facilities include a variety of wind tunnels, structures, and materials laboratories, flight test instrumentation including flight simulators, and a Japanese NEC SX-2 supercomputer. NLR is eager to be involved in cooperative ventures and in doing contract research. The German-Dutch windtunnel, Europe's largest low-speed windtunnel, is also located at NLR's Northeast Polder Facility.

The Netherlands Agency for Aerospace Programs (NIVR). NIVR was founded in 1946 as the Netherlands Agency for Aviation Development. In 1969, its name and function were changed to include space applications. Its function is the promotion of industrial aerospace activities, mainly through contracts for aerospace development projects and technological research programs, and its funding is provided by the government and by a revolving fund, which consists of royalties on technology whose development was financed largely through NIVR. Thus, NIVR gets a payment for each Fokker aircraft built.

Both NIVR and NLR's boards of directors include representatives of the concerned government ministries, universities, the aviation industry, and the Netherlands Organization for Applied Scientific Research (TNO). The government prefers to minimize its direct involvement with industry, though it is willing to fund basic research. It therefore provides NIVR with money, which NIVR then uses to fund research aimed at industrial applications, as well as to partially fund specific development projects in the aerospace sector. NIVR then contracts with NLR or other scientific institution to research a certain problem.

While the government is committed to continued involvement in international space development, its efforts are concentrated on cooperation within the European Space Agency, and on doing contract research for ESA or other interested western parties. NIVR's budget will increase from g120 million ($59 million) in 1987 to g187 million in 1990 and beyond. From this amount, NIVR funds the Dutch contribution to ESA as well as national research efforts. NIVR had requested g235 million by 1990 in order to increase the Dutch stake in the ESA projects, but at present the Netherlands is committed to only a 2.3 percent stake in Ariane 5, a 1.3 percent stake in Columbus, and a 2.2 percent stake in the Hermes projects. In its national research efforts, NIVR funds, on a limited basis, research in advanced propulsion, advanced materials structures, and hypersonic aerodynamics, mainly to "keep in touch."

Professor Gerlach, Chairman of the Board of Directors of NIVR, ascribes government interest in aerospace technology as due to aircraft manufacturer Fokker's presence in the Netherlands. Gerlach believes that market imperfections in the aerospace industry require government intervention to correct. Gerlach also doubts that the commercialization of space will be realized for the majority of countries involved, though he agrees that it must be the goal of all space efforts. Dutch efforts in space are generally in cooperation with ESA (the Dutch also have an ongoing project with Italy to develop an x-ray satellite), and Gerlach sees NIVR's role as assisting in the promotion of technology transfer from space to more general applications.

The Netherlands Aerospace Laboratory. The most unusual feature of the Netherlands Aerospace Laboratory (NLR) is that it gets 70 percent of its income from research contracts and 30 percent of its income from government subsidies and patents. Whereas NIVR generates Dutch aerospace policy, NLR is the primary Dutch research institute focusing on aerospace technologies. NIVR is the single largest customer of NLR's services. NLR itself employs approximately 800 people, of whom 30-odd are working directly on space-related research at any point. About 10-15 percent of NLR's efforts are in space research; the majority of its work is related to aircraft design, primarily for Fokker. Dr. Spee, the Director of NLR, describes NLR's space-oriented research program as aimed at developing the competence within NLR to participate in future aerospace research rather than intended to develop specific technologies. NLR is divided into three administrative divisions and five research divisions: fluid dynamics, flight, structures and materials, space, and informatics. It has two facilities, one in Amsterdam, and another larger complex in the northeast polder (reclaimed land area).

NLR's fluid dynamics division investigates wind tunnel testing techniques, computation aerodynamics (analysis/design), unsteady aerodynamics (flutter), aeroacoustics, propulsion aerodynamics, and wind tunnel instrumentation. Ap-

plied aerodynamic research carried out in cooperation with Fokker emphasizes propeller propulsion, improvement of Aerodynamic efficiency, and aircraft configuration studies.

NLR has four wind tunnels where aerodynamic research can be carried out. The high-speed wind tunnel, a variable-density closed-circuit wind tunnel, measures 2 meters wide by 1.6 meters high. The supersonic wind tunnel, 1.2 meters by 1.2 meters, is a blowdown facility fed by an air storage vessel containing 600 cubic meters of dry air at a maximum pressure of about 400 kPA, with a maximum stagnation pressure of 1470 kPA and maximum running time of 40 seconds. The continuous supersonic wind tunnel, measuring 0.27 meters by 0.27 meters maximum, has a velocity regime ranging from M = 1.2 to M = 6.0. Finally, the low-speed tunnel rounds out NLR's capability to conduct aerodynamic research and also provides it with the capability to conduct nonaeronautical investigations.

NLR acquired a Japanese NEC SX-2 supercomputer in 1987, thus enhancing its ability to do computational fluid dynamics research. NLR estimates that this purchase increased its computational ability by a factor of 100.

NLR's flight division is involved in aircraft/helicopter handling qualities evaluations, performance analysis, aircraft systems and ground equipment, avionics, flight testing, operational research, air traffic control, weapons/stores certification, human factors engineering, and flight simulator applications. NLR has developed a measuring, recording, and processing system (MRVS) for flight testing the Fokker 50 and the Fokker 100 planes. This modular system permits instrumentation packages for specific measuring tasks to be constructed very quickly.

The materials and structures division also supports aircraft projects. Research areas include aircraft loads, structural stability, crack growth/residual strength, dynamic response, fatigue, corrosion, advanced airframe alloys, composite materials and structures, engine materials and coatings, and nondestructive inspection techniques. In conjunction with Delft University and Fokker, NLR contributed to the development of the hybrid composite ARALL (Aramid Aluminum Laminate), and is investigating its applicability as a fuselage skin material. This division is also studying carbon-fiber-reinforced plastics and various aluminum lithium alloys.

NLR's space division in working on the attitude and orbit control system (AOCS) of the x-ray satellite SAX, a bilateral Dutch-Italian project, as well as various ESA/Fokker contracts. It is developing dynamic simulation software for real and non-real time. In the area of thermal control research, NLR is modeling a two-phase system and components, and has developed a void fraction sensor that measures the amount of vapor in a two-phase system. NLR is also involved in telescience research and other areas.

The informatics division of NLR supports the other divisions and does research into production and life-cycle support of information systems. This division has also developed algorithms for data compression and decompression.

Both NIVR and NLR are extremely interested in cooperative efforts. At this point, they are focusing primarily on European space cooperation. NLR is also willing to do contract research for Western interests. Overall, its strength appears to be in the breadth of aerospace research that it can do in a relatively small organization.

Although the German-Dutch windtunnel (DNW) is an independent organization, it too is located at NLR's facility on the northeast polder. The prime facility of this 50/50 cooperative venture between West Germany and the Netherlands is the largest low-speed wind tunnel in Europe, and according to its administrative head, is the top-ranked tunnel in the world for acoustic measurement. It was founded in 1976 and opened in 1980. The tunnel is run with a commercial attitude, and has a high occupancy rate. Last year, approximately 25 percent of its earnings came from US sources.

The DNW has three interchangeable closed test sections of 9.5 by 9.5 meters, 8 by 6 meters, and 6 by 6 meters. The velocity regimes for these test sections range up to 62 m/s, 117 m/s to 153 m/s respectively. Its ventilator has a diameter of 12.3 meters and can function at 225 revolutions per minute. Its primary uses are for research into general low-speed aerodynamics and aeroacoustics, engine airframe interference, rotor aerodynamics, flutter and dynamic testing, optimization of full-scale components, and real engine testing.

Although automobile manufacturers are making less use of this facility as they invest in building their own wind tunnels, the management of the windtunnel is optimistic about its prospects for automobile-related work. They estimate that the future market for the DNW will be 40 percent in civil aircraft, 10 percent in spacecraft, 15 percent in military aircraft, 20 percent in helicopters, and the remaining 15 percent in cars, trucks, and other products. DNW has been used for acoustics research by the US Army and by Boeing, in part, no doubt, because DNW stresses its security arrangements and confidentiality of data. They foresee more opportunities of this nature in the future.

OECD

For further information on items from the Organization for Economic Cooperations and Development (OECD) contact Mr. Robert K. Carr, Office of the Science Counselor, American Embassy, Paris, APO New York 09777.

Three Major European Electronic Groups will Conduct a Joint Research Program on Computer Chips within the EUREKA Framework. The French-Italian Corporation SGS-Thomson, the Dutch group Philips, and the German company Siemens have announced that they will cooperate in equal shares in a joint research program called Jessi (Joint European Semiconductor Silicon) within the EUREKA framework. The three corporations will develop a new generation of large-scale electronic components. Jessi will officially start next year and will include two stages: during the first period (until 1991-1992) industrialists will focus on medium-scale integrated circuits; during the second period (until 1995-1996) industrialists will develop much more sophisticated circuits.

This program requires large-scale financing. It will be necessary to spend at least [French]F2.5 to 3 billion ($400 to 500 million) each year during 7 years. In total, the financing will exceed F20 billion ($3.5 billion). This is the first program of such scope at the European level. The governments concerned (the Netherlands, West Germany, France, and Italy) and the European Community will contribute half of

the funds, the other half to be provided by the industrialists themselves.

Cooperation between European countries appears to be the only way for Europe to catch up with the US and Japan in the area of computer chips. Currently, Europe controls less than 10 percent of the world production of semiconductors, compared with the US whose share represents 39 percent, and Japan which has taken the lead with 48 percent. Furthermore, European manufacturers have not attained the best technological level. Through cooperation, Philips, Siemens, and SGS-Thomson – whose sales in 1987 amounted to $1.6 billion, $657 million, and $860 million respectively – barely attain the level of the first world groups – the Japanese corporations NEC (with a turnover of $3.2 billion) and Toshiba (with a turnover of $3 billion).

The distribution of functions within Jessi was apparently easily resolved. Each partner will concentrate on the areas it is best familiar with. The distribution of responsibilities, however, was not easy. In April, the French and the Italians were concerned that Siemens had announced that themselves and Philips should control the program. Siemens finally accepted to participate in the program in equal shares with the French-Italian group. The latter emphasizes that "cooperation will only concern the development of production processes and not the development of products. Each partner, at this point, will become free again."

The three corporations now have to prove that their cooperation agreement can last. The success of the Jessi program and of the collaboration between governments and industries will also constitute a test for the Europe of 1993.

West Germany

For futher information on items from West Germany, contact Mr. Edward M. Malloy, Office of the Science Counselor, American Embassy, Bonn, APO New York 09080-7400.

West German-USSR Ministerial-Level Agreement on Peaceful Cooperation in Space. On the occasion of Federal Chancellor Kohl's visit to Moscow, the Federal Ministry of Research and Technology and the Soviet Academy of Sciences signed an agreement on October 25, 1988, for scientific and technological cooperation in the research and utilization of space for peaceful purposes. The agreement defines various areas of potential joint research. It focuses on scientific research in solar-terrestrial interactions, space astronomy and astrophysics, investigations of the solar systems, planets and comets, and basic research on mircrogravity, space medicine, and space biology. Other areas of cooperation in space are left open to mutual consent.

According to the agreement, each side assumes the costs of their own research activities. The agreement does not cover projects conducted on a commercial basis. The agreement is limited at first to a 5-year duration but is intended to be extended indefinitely, as long as neither side pulls out. Still incomplete and lacking full accord are the appended lists of projects. The agreement will become effective when the project lists are finalized. The agreement defines regulations about the transfer of information and scientific data, as well as about the liability and medical care for exchanged scientists and experts.

Of course, bilateral scientific cooperation in space between West Germany and the USSR institutes is not new. The agreement provides a framework for existing cooperation and an impulse for expanding the level of German-Soviet cooperation in space. A major innovation of the new interagency agreement is the provision for a German astronaut to be carried on a Soviet mission. Article 2 states:

> "This agreement confirms the understanding already reached between the responsible institutions of the Federal Republic of Germany and the Soviet Union over the participation of a specialist of the other side in a flight on board a Soviet space vehicle and a Soviet orbital space station. The conditions for carrying out this flight will be negotiated between the appropriate institutions of the Federal Republic of Germany and the Union of the Socialist Soviet Republics."

According to press reports, this article caused a lot of difficulties. Early in the negotiations the Soviets sought a payment for the flight opportunity of up to $15 million. West German negotiators firmly rejected this. The first version of the agreement, formulated by the Soviets, would have allowed them to exclude – at least theoretically – a Berlin candidate. In the cabinet discussions on the agreement, the Justice Minister turned the agreement back because the Berlin clause was inadequate – less than a week before the Kohl visit. Mutually acceptable wording was worked out following the so-called Frank-Falin formula. The issue has real significance beyond the politics of Berlin. One of the leading West German astronaut candidates for a Soviet flight would be Reinhard Furrer, a resident of Berlin.

Prometheus – High Tech Research on Drive-Auto-Road Systems. Prometheus is an acronym for a European research initiative entitled "Program for a European Traffic with Highest Efficiency and Unprecedented Safety." A joint undertaking of the European Community and 17 European automobile manufacturers, organized under the aegis of EUREKA, Prometheus seeks to optimize the road transport system in Europe through improvements in both the automobile and the road network. Considered by many as EUREKA's most important project, Prometheus employs over 300 scientists from the five automobile producing nations (Germany, the UK, Sweden, France, and Italy) and has a budget of DM1.3 billion ($730 million) until 1994. Some examples of the programs under development are: making road traffic information available to the driver via an onboard computer to assist in route planning, automatic communication between vehicles giving advance warning of hazardous road conditions, stalled traffic, or accidents ahead, and eventual formation of "road-trains" consisting of electronically linked cars traveling at high speed and close quarters on the autobahn to maximize highway efficiency.

Prometheus was initially suggested by the German automobile manufacturers (Daimler-Benz, Volkswagen/Audi, Porsche, and BMW), and has been expanded to include the major (non-American) automobile firms in Europe.

The German automobile industry will contribute DM420 million ($236 million) to the overall budget of DM1.3 billion ($730 3 million) which will run until 1994. Prometheus is not focused primarily on the competitive aspects of a car's performance. Thus, it will not subsidize the development of the next generation of automobiles by conducting research into

high-performance engines or electronic engine management. Rather, the concept behind Prometheus is to further the cooperation between industry and government so that governments develop "smart roads" to coincide with the "smart car" of the future, along with making any necessary adjustment to traffic laws, to accomplish an overall improvement in the road traffic network.

The environmental impact of road traffic is a major problem. The Environmental Ministry estimates that road traffic accounts represents the following percentage of all air pollution in West Germany (figures in metric tons):

57.9 percent of CO_2 (4.31 million tons)
54.0 percent of NO_2 (1.65 million tons)
42.9 percent of hydrocarbons (0.8 million tons)
10.1 percent of dust caused by human activities, especially diesel particulates (66,000 tons)

An additional factor is the noise of road traffic, considered by some 42 percent of all households as the biggest factor in pollution caused by cars and trucks.

The solution offered by Prometheus is to capitalize on recent advances in microelectronics, sensor technology, telecommunications and informatics to provide onboard technical systems which, with corresponding roadside equipment, would give information about present road and traffic conditions, recommend routes, give advice on how to drive and warn of dangers. For example, fog conditions often lead to multiple pile-ups on the autobahns involving as many as 100 vehicles. Were the first damaged car equipped with an automatic warning system and following vehicles capable of receiving this warning they could be braked in time to avoid the pile-up. Lack of knowledge about road and traffic conditions on the part of the driver can be compensated by an interactive system between cars and the overall traffic management system, provided by roadside equipment. Alternative routings can be suggested by the traffic computer reducing the overall congestion on any part of the road traffic system.

Prometheus is structured into seven component programs.

- "Pro-car" deals with improvements in the car itself, such as antilock braking and trip computers. This is the area where most rapid progress is foreseen.
- "Pro-net" involves automatic communication between vehicles, such as warnings of congestion ahead which would signal to brake.
- "Pro-road" represents communications between vehicle computer and traffic computer, providing information such as updates on road traffic and conditions.
- "Pro-chip" is the development of microelectronics which can be used in vehicles in an artificial intelligence system in the onboard computer, and
- "Pro-com" seeks to develop the structures and standards for data exchange necessary for communication between vehicle and environment as well as component interfaces.

In conjunction with Prometheus is an EEC initiative called "DRIVE" (dedicated road infrastructure for vehicle safety in Europe), which focuses on development of the road system rather than the vehicle. Research undertaken by DRIVE will include compiling accident data, developing transmission technologies, traffic sensors, and radar systems, and utilizing software for infrastructure planning, traffic management, traffic modeling, and development of strategies for traffic management. The DRIVE program will be guided by the analysis of road users and transport administrators requirements with a research and development work targeted to assist in the implementation of this overall strategy. Cost of DRIVE is estimated at 60 million ECU $70.2 million) over 3 years, with a special provision that expenditure on staff not exceed 4.5 percent of the total costs.

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